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PORTABLE COMPUTING SYSTEM FOR USE IN TOXIC GAS EMERGENCIES

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Ontario
Ministry of the Environment

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PORTABLE COMPUTING SYSTEM FOR

USE IN TOXIC GAS EMERGENCIES

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The Ministry of the Environment takes no responsibility whatsoever for any outcome resulting from use of this report or computer program.

SUMMARY

This report serves as the documentation for the portable computing system for use in toxic gas emergencies. This system has been developed and is maintained by the Atmospheric Contaminants and Research Planning Unit of the Air Resources Branch. The main objectives are:

a) a system which can provide hazardous contaminant and dispersion modelling information quickly in an emergency.

b) a system which is "user friendly" to inexperienced users.

c) a system which is easily transportable so that it can be used at home or at emergency sites.

The report is written in modules so that readers of different sophistication in computer modelling of toxic gas dispersion can use different parts of the report. Chapter 1 spells out the rationale for developing the system and the scope of its intended use. Chapter 2 provides some background information on the modelling calculations and the information sub-system. Chapter 3 is a User's Manual, giving step-by-step instructions as to how to use the system. Chapter 4 contains flow charts showing the system design as well as the data structure of the files making up the information sub-system.

The programs and further documentation can be obtained from:

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CHAPTER 1: INTRODUCTION

1. INTRODUCTION

Storage, handling and transportation of hazardous gases are necessary because of their extensive use in our industrial society. Toxic gases such as ammonia, chlorine and hydrogen sulfide are stored in refrigerated vessels or pressurized tanks and are transported by ship, truck, or train.

The manufacturers and shippers of these materials do their best to ensure that the materials are stored and moved safely and that hazards due to toxic properties of these materials are minimized. A great variety of failure mechanisms, however, can sometimes disrupt our lives. People living in Toronto and Mississauga may remember the train derailment in 1979. A quarter of a million people were evacuated and police, firefighters, meteorologists, hospital staff, ambulance crews, and environmental scientists all played critical roles in handling the emergency. In 1982, a train derailment at Medonté, near Barrie, Ontario, threatened the surrounding community with the potential rupture of a tank car containing 39 tons of anhydrous hydrogen fluoride. In other countries lives have been lost in such accidents.

In 1980, the Ontario Ministry of the Environment started to develop computerized dispersion models to calculate the estimated concentration of toxic gases resulting from unusual releases to the atmosphere. These models were developed on an IBM mainframe computer. The models were to be used by the appropriate authorities to help in decision making about evacuation of people in the general area of the accident. When major emergencies occur at unusual hours (as often happens), these programs can be run on a terminal from the home of MOE staff via telephone line. If the user requires his phone line to run these models, however, his communication line is cut off. If the mainframe is down for maintenance or for some other reason, these models cannot be used.

To avoid such situations, the Ministry of the Environment has adapted the Simple Gas Model and the Heavy Gas Model to a portable computer (Osborne 1). The resulting system also contains useful information on 79 priority chemicals which might be involved in emergencies in Ontario. The portable computer can be brought to the emergency site and used there. If kept in the homes of personnel on a rota basis, it can also be used to provide a fast information response when major emergencies occur at unusual hours.

This portable computing system for use in toxic gas emergencies (henceforth referred to as the GAS SYSTEM) is designed to be very user-friendly so that a minimum of computer competency is required to run the system. It is not meant to replace the professional dispersion modeller. Rather, its main purpose is to provide fast, first-cut information to advise appropriate emergency handling authorities at the emergency site. The system will provide hazardous contaminants information, calculate toxic gas concentrations at different distances downwind of an emergency site, and display this information graphically against important marker levels such as TLV, STEL and IDLH values (Threshold Limit Values; Short Term Exposure Limits; Immediately Dangerous to Life or Health). This information will aid authorities in decision making about evacuation of people in the general area of the crash. Meanwhile, professional modellers from industry and government can set up more detailed models for the particular circumstances.

CHAPTER 2: BACKGROUND

2.0 BACKGROUND

2.1 FORMATION OF HAZARDOUS VAPOUR CLOUDS

The accidental escape of chemicals during manufacture, storage, and transportation can harm the public. The understanding of the atmospheric dispersion of toxic vapours is, therefore, an essential element in chemical safety plans. One of the most important properties of such vapours is that many of them are denser-than-air. Many other vapours, although not normally denser-than-air, may become so under typical emergency conditions. Following are some surprising examples of denser-than-air behaviour for gases that, at first sight, should be buoyant. This is important because such gases will tend to remain near the ground while moving downwind, thus increasing the risk in the downwind area.

Gases can be intrinsically dense because their molecular weight exceeds that of air. Chlorine is an example of a dense toxic vapour. The petrochemical industry produces and transports a range of flammable dense hydrocarbons such as propane, butane, and propylene. Although methane is a gas whose molecular weight is less than that of air, it is dense if released at its boiling point of -161°C. Natural gas is often stored or transported as liquid and a cold, dense vapour can be generated if liquified natural gas should be spilled onto land or water.

A superficially surprising example of a gas that can form a denser-than-air mixture is ammonia, which is chemically toxic. Its molecular weight is only 17 and, at its boiling point of -33°C, the vapour is less-dense-than-air at 20°C. Nonetheless, there are several examples of accidental releases of ammonia from pressurized containers in which the resulting gas cloud was denser-than-air (Kaiser and Walker, 1978), or at least non-buoyant. The reason for this is as follows. If ammonia is kept as a liquid at the ambient temperature, it is under considerable pressure. If the vessel containing the ammonia should fail, there is an immediate bulk boiling of the liquid. About twenty percent of its mass can typically vaporize, with the heat supplied by cooling the remaining ammonia to its boiling point. The vigour of the bulk boiling process can throw most, if not all, of the remaining liquid into the air as a fine aerosol. At the same time, air is entrained. This air supplies heat to evaporate the ammonia droplets so that a mixture of air and ammonia, possibly at the boiling point of ammonia, is formed. Such a mixture can be denser than the surrounding air, if the circumstances favour the release of a substantial

percentage of the ammonia as fine liquid droplets. Such a case occurred in the USA in May, 1976. Nineteen tons of anhydrous ammonia were released in a dense cloud in surburban Houston when a truck tanker crashed through a barrier on an elevated expressway.

Another example is hydrogen fluoride, a toxic gas used by the nuclear industry during the fuel manufacturing process and by the chemical industry as a catalyst in alkylation plants. Its molecular weight is normally 20, but as a pure vapour it is highly associated and consists of a mixture of a hexamer and monomer with an effective molecular weight of about 70. Dissociation takes place as the hydrogen fluoride is diluted with air, but the heat required to do this is extracted from the mixture and tends to keep it denser than the surrounding air. However, there is no known example of a large scale accidental release in which this density effect has been observed.

From the foregoing examples, it is apparent that a knowledge of the way in which "heavy" toxic vapours disperse in the atmosphere is essential to analyse the potential risk in accidents involving toxic chemicals.

2.2 DISPERSION MODELS

After the release of a toxic vapour, its concentration at different distances downwind can be estimated using dispersion models. The purpose of the dispersion calculations presented in this portable computing system is to obtain a rough estimate of the dispersion of hazardous vapour. Various simplifying assumptions are incorporated into models of different sophistication. The reader should be aware of the inherent assumptions and the limits of applicability of these models. Otherwise, gross misinterpretation of the implications of a particular situation may result. For instance, the terrain is assumed to be flat. In a real situation, channelling due to buildings or valleys can lead to higher concentrations than predicted.

The accidents dealt with can be subdivided into two major types:

a) Continuous Release (Plume Formation) - A leak occurs in a gas container or above the liquid level in a liquid container. Alternatively, liquid is released, forms a pool and evaporation causes vapour release to the atmosphere.

b) Instantaneous Release (Puff Formation) - This is the release of a large amount of gas in a very short time (in the order of seconds to minutes). A major rupture in a container of a highly volatile chemical can cause such a release, e.g. a BLEVE (Boiling Liquid Expanding Vapour Explosion).

Two types of dispersion model have been incorporated in the present system. The Simple Gas Model can deal with either a continuous or instantaneous release and uses different equations to estimate the concentration downwind for these two situations. The Heavy Gas Model, although a more mathematically sophisticated model, can only deal with instantaneous releases in our system. It will give a more realistic representation of an instantaneous heavy gas release.

2.3 SOURCE STRENGTHS

The use of these models requires that the amount of gas released (i.e. source strength) be known. Source strengths can be estimated using basic principles of thermodynamics and fluid mechanics. In the development of the following formulae, gases are assumed to behave ideally and the venting process is assumed to be isothermal. Equilibrium thermodynamics, although not strictly applicable, is employed for simplicity. These assumptions may not be valid in many cases, but they do give a worst-case scenario.

2.3.1 Gas Release

Gas will be released when the hole in the tank is above the liquid level. The maximum limiting flow rate for gas release is during "choked" flow. This flow rate is

$$q_v = C_d A P \sqrt{\left(\frac{KM}{RT}\right)\left(\frac{2}{K+1}\right)^{\frac{K+1}{K-1}}}$$

where q_v = vapour venting rate
T = absolute temperature in the tank
M = molecular weight
R = universal gas constant
P = tank pressure
K = specific heat ratio for the vapour
C_d = coefficient of discharge
A = area of rupture

The criterion for choked flow is

$$\frac{P}{P_a} > \left(\frac{K+1}{2}\right)^{\frac{K}{K-1}}$$

where P_a = atmospheric pressure.

For unchoked flow,

$$\frac{P}{P_a} \leq \left(\frac{K+1}{2}\right)^{\frac{K}{K-1}}$$

and the flow rate becomes

$$q_v = C_d A \sqrt{2P\rho_v \left(\frac{K}{K-1}\right)\left\{\left(\frac{P_a}{P}\right)^{\frac{2}{K}} - \left(\frac{P_a}{P}\right)^{\frac{K+1}{K}}\right\}}$$

where ρ_v = density of vapour.

2.3.2 Liquid Release

Liquid is released when the hole in the tank is below the liquid level. Then,

$$q_\ell = C_d A \rho_\ell \sqrt{2gH + \frac{2(P-P_a)}{\rho_\ell}}$$

where q_ℓ = instantaneous liquid venting rate
H = height of liquid column above hole
P = tank pressure
A = area of rupture
C_d = coefficient of discharge
ρ_ℓ = density of liquid
g = acceleration due to gravity
P_a = atmospheric pressure

Stiver and MacKay (1982) give the evaporation rate for chemicals that form a liquid pool when spilled on a ground or water surface as:

$$Q = \frac{K_m A_p P M}{RT}$$

where Q = evaporation rate (vapour release rate), kg/s
K_m = mass transfer coefficient, m/s
A_p = pool area, m^2
P = vapour pressure, Pascal (i.e. N/m^2)
M = molecular weight
R = gas constant, 8.314 $(Pa)(m^3)/(mole)(^oK)$
T = temperature, ^oK

At a temperature of 20°C, the evaporation rate can be given numerically as

$$Q = 8.5 \times 10^{-10} A_p P M u^{0.78} \text{ kg/s}$$

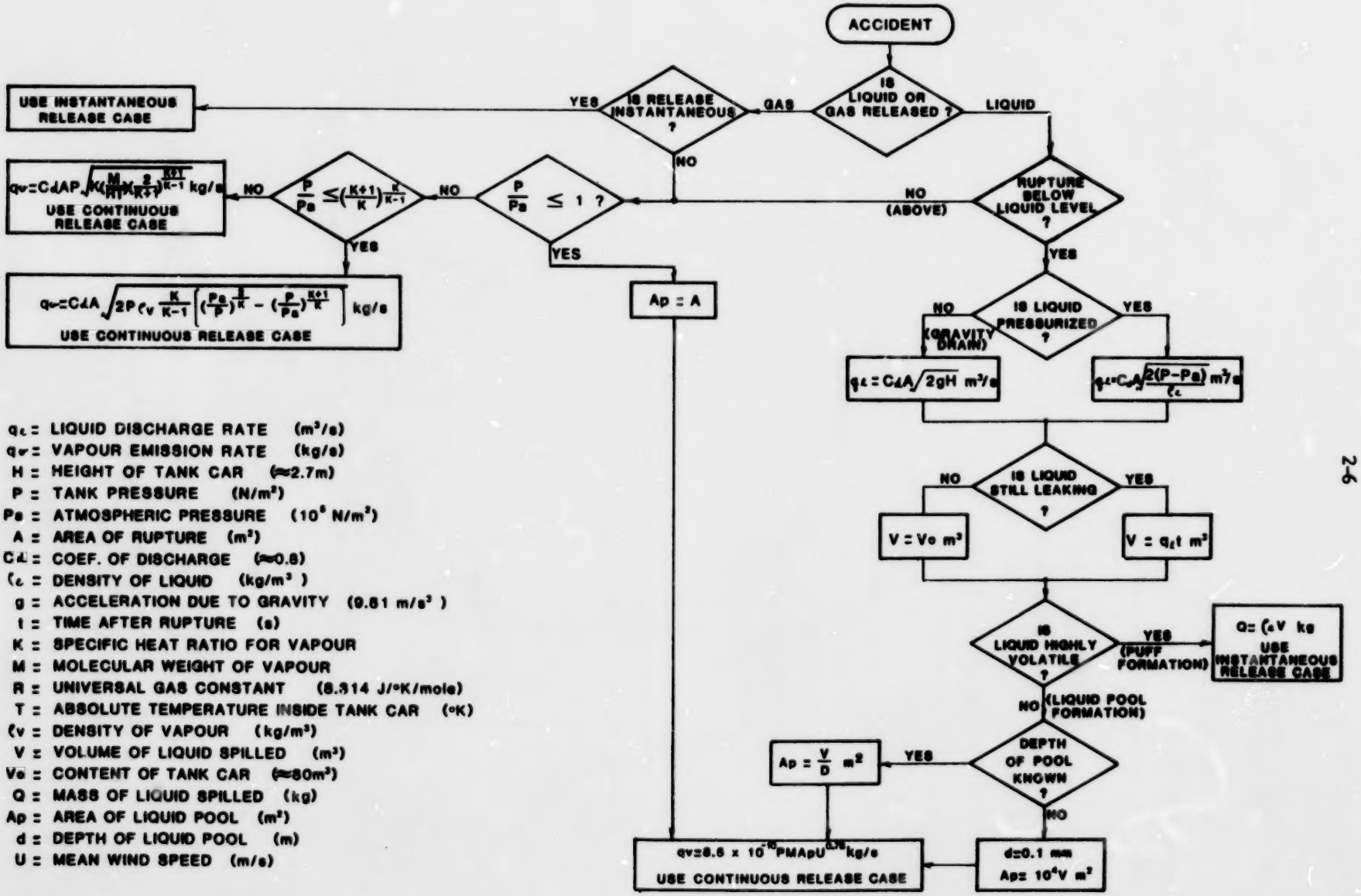
where u = the wind speed in m/s.

The evaporation rates at temperatures other than 20°C use the following equation:

$$Q_t = Q_{20^oC} \times \frac{P_t}{P_{20^oC}} \times \frac{T_{20^oC}}{T_t}$$

where the subscript t denotes the temperature at which the evaporation rate is desired.

The accompanying flow chart shows how the computer program determines the release rate of toxic gases in an accident.



q_ℓ = LIQUID DISCHARGE RATE (m³/s)
q_v = VAPOUR EMISSION RATE (kg/s)
H = HEIGHT OF TANK CAR (≈2.7m)
P = TANK PRESSURE (N/m²)
Pa = ATMOSPHERIC PRESSURE (10^5 N/m²)
A = AREA OF RUPTURE (m²)
C_d = COEF. OF DISCHARGE (≈0.8)
ρ_ℓ = DENSITY OF LIQUID (kg/m³)
g = ACCELERATION DUE TO GRAVITY (9.81 m/s²)
t = TIME AFTER RUPTURE (s)
K = SPECIFIC HEAT RATIO FOR VAPOUR
M = MOLECULAR WEIGHT OF VAPOUR
R = UNIVERSAL GAS CONSTANT (8.314 J/°K/mole)
T = ABSOLUTE TEMPERATURE INSIDE TANK CAR (°K)
ρ_v = DENSITY OF VAPOUR (kg/m³)
V = VOLUME OF LIQUID SPILLED (m³)
Vo = CONTENT OF TANK CAR (≈80m³)
Q = MASS OF LIQUID SPILLED (kg)
Ap = AREA OF LIQUID POOL (m²)
d = DEPTH OF LIQUID POOL (m)
U = MEAN WIND SPEED (m/s)

2.4 SIMPLE GAS MODEL

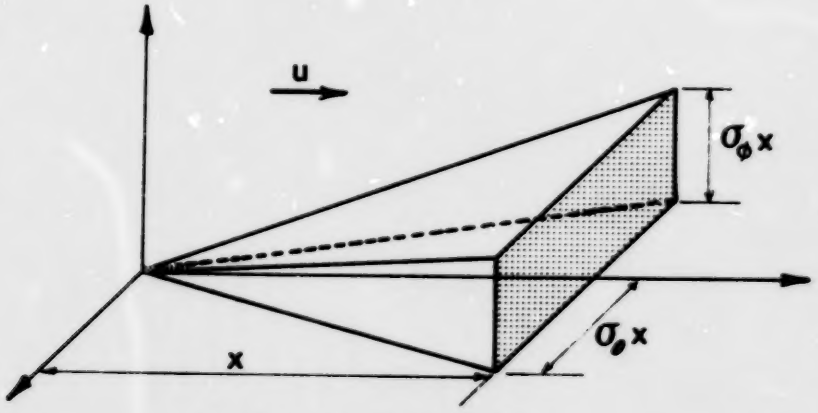
This model is essentially a simplified mathematical description of the physical behaviour of the released gas. In its simplest form, the model expresses the mass balance of the released gas.

In using the puff and plume equations described below, the following assumptions have to be noted (from TIPS Manual, Environment Canada):

a) The vapour that is diffusing is neutrally buoyant; that is, there is no gross movement of the vapour cloud caused by either gravity or buoyancy.
b) Mixing with air is uniform throughout the vapour cloud.
c) The concentration obtained is time-averaged.
d) The wind is uniform throughout the vertical extent of the cloud.
e) The terrain is assumed flat (i.e. no terrain effects).
f) No depletion of the puff/plume (e.g. by deposition).

2.4.1 Continuous Release Case (Plume), Simple Gas Model

Consider a continuous release of gas at a rate of Q at ground level. Plume behaviour can be simplified as a half-pyramid with the apex at the source. Figure 1 illustrates this.



u : MEAN WIND SPEED
x : DOWNWIND DISTANCE FROM THE SOURCE
σ_ϕ : VERTICAL FLUCTUATION
σ_θ : HORIZONTAL FLUCTUATION

Figure 1

If we consider the shaded cross-section, the conservation of matter can be stated as

$$Q = 2\sigma_\theta x \sigma_\phi x u C \qquad (1)$$

where C is the concentration of the gas at distrance x. Formula (1) can be rewritten as

$$C = \frac{Q}{2\sigma_\theta x \sigma_\phi x u} \qquad (2)$$

We can see that:

i) the concentration is directly proportional to the emission rate Q;

ii) the concentration is inversely proportional to the wind speed u; and

iii) the concentration falls approximately as x^2.

The height of the plume in the atmosphere cannot exceed the mixed layer height, z. When the plume height reaches z, the plume will spread horizontally only, instead of both horizontally and vertically (Figure 2).

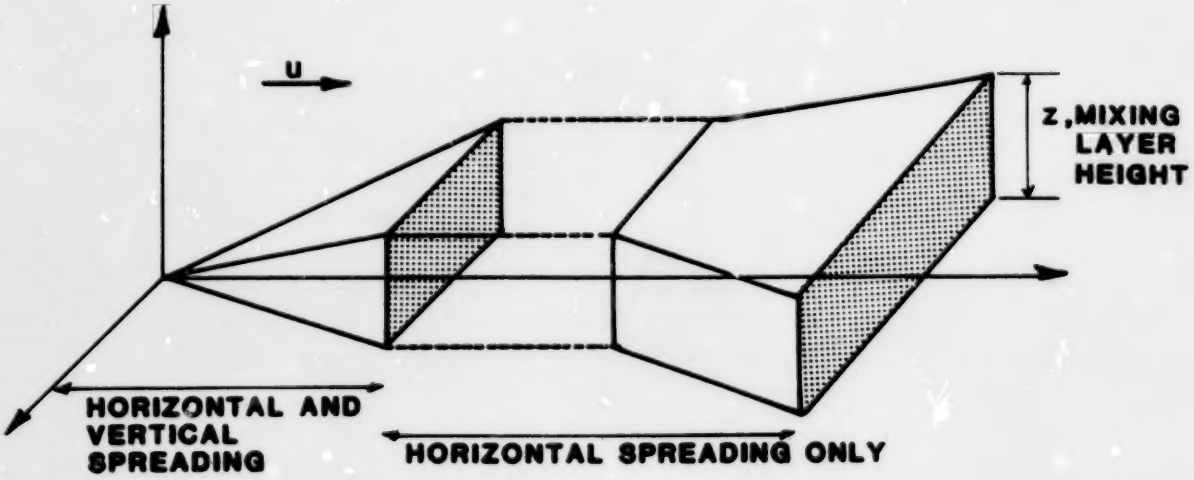


Figure 2

Equation (2) now becomes

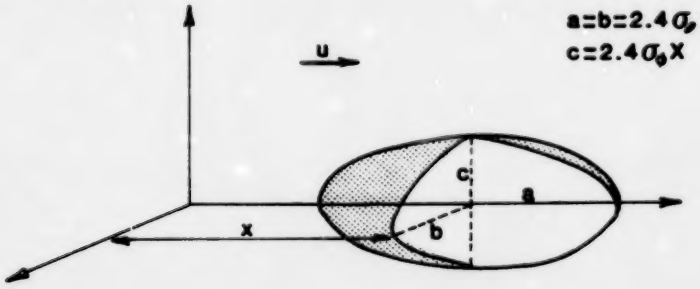
$$C = \frac{Q}{2\sigma_\theta x \sigma_\phi x u} \quad , \sigma_\phi x < z \tag{3a}$$

$$C = \frac{Q}{2\sigma_\theta x z u} \quad , \sigma_\phi x \geq z \tag{3b}$$

Using equations (3a) and (3b), the maximum permissible emission rate or a caution distance can be calculated, provided that the critical concentration is known.

2.4.2 Instantaneous Release Case (Puff), Simple Gas Model

The total mass (W) of the gas is considered to be contained in an ellipsoidal puff, as illustrated in Figure 3, moving along with the wind at a speed u.



u : MEAN WIND SPEED
x : DOWN WIND DISTANCE FROM THE SOURCE
σ_ϕ: VERTICAL FLUCTUATION
σ_θ: HORIZONTAL FLUCTUATION

Figure 3

Then conservation of mass requires that

$$C = \frac{2W}{(2\pi)^{3/2}(\sigma_\theta x)^2 \sigma_\phi x} \quad , \sigma_\phi x < z \tag{4a}$$

$$C = \frac{2W}{(2\pi)^{3/2}(\sigma_\phi x)^2 z} \quad , \sigma_\phi x > z \qquad (4b)$$

where C is the concentration of the gas at the centre of the puff and z is the mixing layer height.

The time of exposure to the puff at a distance x downwind from the source is the time taken for the ellipsoid to pass through.

$$\text{Time of exposure} = \frac{4.8\sigma_\theta x}{u} \qquad (5)$$

If a critical concentration is given, equations (4a) and (4b) can be reversed to calculate a caution distance.

2.5 HEAVY GAS MODEL

In the present system, the heavy gas model can only be used for instantaneous releases. In some cases the hazardous gas is released in a very short time interval (i.e. practically instantaneous). Chlorine escaping suddenly from a fractured pressured vessel is a typical example. The gas appears in the form of a cloud which drifts downwind as it disperses. Figure 4 shows a schematic of a dispersing puff.

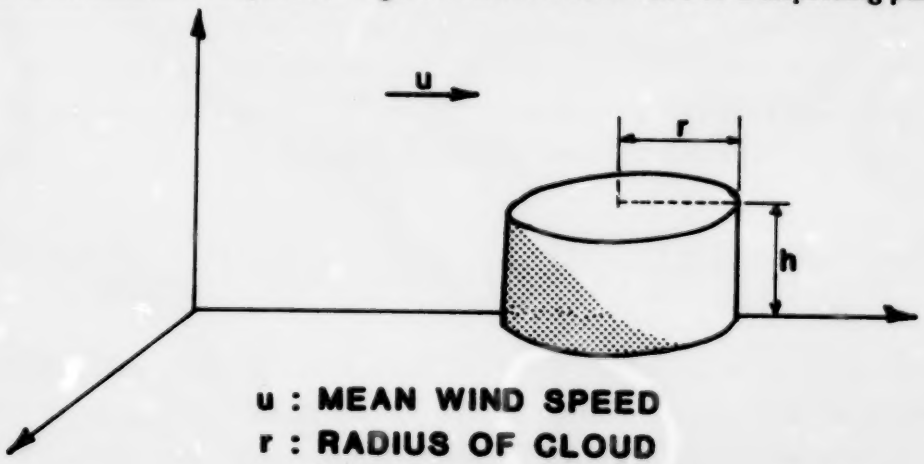


Figure 4

2.5.1 Cloud Formation

The fraction, δ, of the liquid mass thrown into the air-gas mixture as droplets during the release evaporates. Depending upon the type of gas and release, this fraction may vary from almost zero to close to one. A typical value is 0.8 (Kaiser and Walker, 1978). The temperature of the cloud will not rise much until enough warm air has been entrained to evaporate the droplets. The necessary amount of entrained air is

$$M_{ad} = \frac{\delta M_g L_g}{C_{pa}(T_a - T_g) + L_w X_w} \tag{6}$$

Here X_w is the mixing ratio of water vapour, L_w is the latent heat of evaporation or sublimation of water, M_g is the mass of the released gas, and L_g is the latent heat of the gas (K.J. Eidsvik, 1979). C_{pa} is the heat capacity (1005.7 J/kg) of air, which will be cooled during the evaporation process from ambient temperature T_a to T_g, usually the boiling point of the gas.

Since the mass of air entrained is assumed to be ten or twenty times that of the gas in the escaping puff, the law of conservation of momentum dictates that the initial velocity is roughly that of the surrounding air. The puff is assumed to move with the wind speed (measured at a height of 10 m).

2.5.2 Slumping

The initial spreading of the dense cloud resulting from a heavy gas release is controlled by gravitational effects. The cloud essentially slumps under the influence of gravity. To analyze this behaviour, we have followed Kaiser and Walker (1978) and assumed that the cloud is in the form of a cylinder with a radius r and height h. The velocity of the edge of the cloud is adequately described by the liquid column analogy:

$$\frac{dr}{dt} = C\left(\frac{\rho - \rho_a}{\rho} gh\right)^{\frac{1}{2}} = \frac{C}{r}\left(\frac{(\rho - \rho_a) g V_o}{\pi \rho}\right)^{\frac{1}{2}} \tag{7}$$

where dr/dt is the spreading velocity of the cylinder of heavy gas, ρ is the density of the gas-air mixture in the cloud, ρ_a is the density of the surrounding air (1.2 kg/m^3 at 20°C), and C is a constant. Van Ulden (1974) suggested C = 1 as the constant with his field experimental results. We have

also assumed that the volume and the concentration of the cloud remains approximately constant, at V_o and C_o respectively, as the cloud slumps. Integrating equation (7) gives

$$r^2 = r_o^2 + 2\left(\frac{(\rho-\rho_a)gV_o}{\pi\rho}\right)^{\frac{1}{2}} t \tag{8a}$$

$$\frac{dr}{dt} = \frac{1}{r}\left(\frac{(\rho-\rho_a)gV_o}{\pi\rho}\right)^{\frac{1}{2}} \tag{8b}$$

$$C_o = \frac{M_g}{V_o} \tag{8c}$$

Since the concentration remains essentially unchanged at its initial value throughout the slumping phase, exposure levels could be exceedingly high at distances of the order of a few kilometers from the release site.

2.5.3 Termination of Slumping

Slumping is terminated by entrainment of air. This results in a dense cloud which hugs the ground as it travels downwind and the height of the cloud begins to grow at a slow rate. Sooner or later the cloud of dispersing gas must become so dilute that atmospheric turbulence becomes dominant in controlling cloud growth. Van Ulden (1974) recommends as a criterion for the end of the slumping phase to set the turbulence energy density equal to the mean potential energy density; that is to say

$$\frac{1}{2}(\rho-\rho_a)gh = 2\rho u_*^2 \tag{9}$$

Here u_* is the friction velocity due to mechanical turbulence and is related to the mean wind speed u by $u_* = cu$, where c is a "surface drag constant" that depends on the weather category.

Applying equation (7), this criterion is equivalent to

$$\left(\frac{(\rho-\rho_a)gh}{\rho}\right)^{\frac{1}{2}} = \frac{dr}{dt} = 2u_* \tag{10}$$

Combining equations (8b) and (10), the radius at the end of the slumping phase can be shown to be

$$r_t = \frac{D}{2u_*} \quad \text{where} \quad D = \left(\frac{(\rho-\rho_a)gV_o}{\pi\rho}\right)^{\frac{1}{3}} \tag{11}$$

Then the duration of the slumping phase is given by equation (8a) as

$$t_T = \frac{r_T^2 - r_o^2}{2D} \tag{12}$$

After $t = t_T$, dr/dt becomes independent of r. To be consistent with equation (10), $dr/dt = 2u_*$ and

$$r = r_T + 2u_*(t-t_T) \tag{13}$$

Similarily, for the growth of cloud height, Eidsvik gives

$$h = h_T + \alpha u_*(t-t_T) \qquad \text{for} \quad h < z \tag{14}$$

where α is a coefficient for vertical entrainment with a value of about 0.4.

2.6 INFORMATION SUB-SYSTEM

In addition to the source strength programs and modelling programs the computer contains an information sub-system. This sub-system contains physical and chemical data on 79 priority chemicals. In a previous MOE report "Atmospheric Monitoring for Transportation Emergencies" (ARB-030-81), these 79 chemicals were identified as posing the highest risk to human health and the

environment from transportation-related spills in Ontario. These chemicals were selected by considering the inherent toxicity of the chemical or its products, and the probability of its being involved in a spill in Ontario.

For each chemical, the following physical and chemical data are stored in retrievable form:

i) Formula

ii) Molecular weight

iii) Latent Heat of Vapourization (or Sublimation)

iv) Boiling Point - measured at 1 atmosphere

v) Solubility - measured at 0°C unless specified inside brackets

vi) Specific Gravity - with respect to 4°C water at 1.00. (If gaseous, the value reported is that of the liquid at a common compressed state.)

vii) Vapour Pressure - saturated vapour pressure measured at 20°C unless otherwise specified inside brackets

viii) Vapour Density - with respect to air at 1.00.

ix) Flash Point - measurement method coded inside brackets
(CC) closed cup method
(OC) open cup method

x) IDLH - Immediately Dangerous to Life and Health concentration
This is usually defined as a thirty minute exposure. It is used as a guide in the industrial situation as a concentration from which workers would not be able to safely escape if their respiratory equipment failed.

xi) TLV - Threshold Limit Values (Time Weighted Average)
This is defined as the time weighted average concentration for a normal 8-hour workday and a 40-hour workweek, to which nearly all workers may be repeatedly exposed, day after day, without adverse effect.

xii) STEL - Short Term Exposure Limit
This is defined as a 15-minute time-weighted average exposure which should not be exceeded at any time during a workday even if the eight-hour time-weighted average is within the TLV.

xiii) Specific Heat Ratio - ratio of specific heats of the vapour at constant pressure and at constant volume

xiv) Synonyms - different names for the same chemical

xv) Fire Hazards Code - describes the flammability or combustibility of the chemical and any special hazards posed by its combustion or behaviour in a fire, including toxic products or potential for explosion.

2.7 SYSTEM OUTPUT

The output from the information sub-system is combined with the model calculations to give useful information on potential concentrations of toxic gases downwind of a release. If a critical concentration for human health is entered into the system, a "caution distance" will be calculated. If actual measurements of toxic gas concentrations are made at the site, an emission rate may be estimated.

The Simple Gas Model output can be graphically displayed on the computer terminal, showing downwind concentration in context with TLV and IDLH levels (Threshold Limit Values and Immediately Dangerous to Life and Health values).

The Heavy Gas Model output can be printed on a portable printer and this output is given for a series of different downwind distances.

CHAPTER 3: USER'S MANUAL

3.0 USER'S MANUAL

3.1 THE OSBORNE 1

3.1.1 Setting up the Osborne 1 Computer (blue case)

1) Place it on a flat surface with the two black plastic latches facing up. Slide open the ventilation window on the top side.

2) The keyboard is on the inside of the cover, which you remove by unfastening the latches. The keyboard is connected to the main body of the Osborne 1 via a cable. BE CAREFUL that you do not jerk the keyboard away from the computer; doing so may damage the cable.

3) Plug in the removable power cord and connect it to a 110V AC power source. The power switch is located in the recessed cavity at the back of the machine. Turn the power on. You should hear a beep.

4) A sign-on message will appear on the monitor (display screen) after a few seconds. If not, see whether the brightness and contrast controls are well adjusted. Try "twiddling" the knobs labelled "BRT" (for brightness) and "CONTR" (for contrast) as you would on a television set. Now, the computer is ready for use. Follow the instructions in Section 3.2, but make sure you understand the following information on the handling of program diskettes.

3.1.2 Disk Drive Operations

The Osborne 1 has two disk drives, one on each side of the monitor. The one on the left is called drive A and the one on the right is drive B.

The program diskettes are thin plastic disks with a magnetic coating. They must be removed from the paper pocket before using. But NEVER try to get the plastic disk out of the blank vinyl envelope.

NOTE: This Osborne 1 computer generates and uses radio frequency energy, and if not installed and used properly it may cause interference to radio reception.

PUTTING DISKETTES INTO THE DRIVES

1. The disk drives have little doors that are like small flaps. If not open already, open the door by gently lifting the flap.

2. Insert the diskette into the drive, making sure that the label is on the top and facing outward.

3. Close the door.

REMOVING DISKETTES FROM THE DRIVES

1. Flip the door open and gently pull the diskette out.

2. Do not bend the diskette when inserting or removing it.

3. NEVER ATTEMPT TO REMOVE A DISKETTE from a drive while the disk activity light is on. The disk activity light is a small red light beneath the drive. If you remove the diskette when the light is on, you will lose the program.

DISKETTE HANDLING

1. It is very easy to damage a diskette's surface and lose the information stored on it.

2. Avoid placing the diskette near any magnetic field (this erases all the information).

3. Keep all exposed surfaces protected from dust and contact with other foreign materials. Keep the diskette inside its paper pocket unless it is being used in the drive.

4. Store diskette in a cool, clean, dry place.

5. Do not touch the magnetic surface with your fingers.

6. NEVER turn the power on or off while diskettes are in the drives. Doing so may destroy the stored information.

3.2 GAS SYSTEM

3.2.1 Set Up Procedure

GAS SYSTEM consists of several MBASIC programs and some data files. They are stored in two diskettes. To start the system, follow the following instructions:

1) Make sure that the Osborne 1 is on.
2) Insert Diskette A into Drive A (the one on the left).
   Insert Diskette B into Drive B (the one on the right).
3) Press the RETURN key to load the MBASIC interpreter. When finished, an 'OK' message will appear as the last line on the screen.
4) Press Control-1 (press 1 while the CTRL key is held down),
   Or type RUN "GAS" and press the RETURN key.
5) You will see the following display on the screen. Choose the program you want to run by pressing a number between 1 and 3.

```
****************************************
*                                      *
*          GAS  SYSTEM  MENU           *
*                                      *
****************************************


   TYPE   1.  FOR INFORMATION ACCESS

          2.  FOR SIMPLE GAS MODEL

          3.  FOR HEAVY GAS MODEL

          4.  EXIT TO MBASIC
```

On entering the GAS SYSTEM, you MUST press 1 to ensure that information on the chemical you want is stored for your current use.

6) Follow the instructions on the following sections for running the different models or programs.
7) When finished and this GAS SYSTEM MENU reappears on the screen, press 4 to exit the GAS SYSTEM.
8) Remove the program diskettes and put them back into their paper pockets before storing.
9) Turn the Osborne 1 computer off.

3.2.2 Normal Operation Steps in Case of Emergency

1) Run the Information Sub-system to look for the chemical in question. The system will store the properties of the located chemical onto a data file (named B:JINFO.DAT) for later access by the Simple Gas Model and the Heavy Gas Model. If the chemical is not one of the 79 stored, consult other emergency response handbooks.

2) Run the Simple Gas Model. The system will ask whether you know the source strength. If you answer yes, the Simple Gas Model Menu will be presented. Otherwise, the system will lead you through the routine to estimate the source strength (See Section 2.3). The system will use this value as default value for emission or emission rate in the appropriate simple gas dispersion calculation.

3) If the release is instantaneous and the circumstances permit, you can run the Heavy Gas Model to obtain a more realistic estimate of concentration versus downwind distance.

WARNING:

If step 1 is bypassed, the information on the chemical last accessed will be used for subsequent computations. THIS MAY NOT BE THE ONE YOU WANT.

3.3 INFORMATION SUB-SYSTEM

The Information Sub-system consists of a set of programs and files (See Chapter 4) to provide information on physical and chemical properties of 79 hazardous chemicals. The system consists of 4 routines:

Display Routine
Add Routine
Modify Routine } Entry requires valid password
Change Routine

DISPLAY ROUTINE displays selected physical and chemical properties, synonyms, and fire hazard codes of the requested chemical compound if it is in the Information File.

ADD ROUTINE is used to enter a new chemical compound into the Information File. The user must provide all information in standard units displayed.

MODIFY ROUTINE allows the user to add physical or chemical properties to all the records in the Information File.

CHANGE ROUTINE allows a user to change the value of one or more fields of the requested chemical; or to put in the value of a new field added by the MODIFY ROUTINE.

WARNING:

Take extreme care while running the ADD and MODIFY routines. They alter the file structure and mistakes cannot be easily undone.

3.3.1 Getting Into Routines

After pressing 1 at the GAS SYSTEM MENU and shortly after a **"PLEASE WAIT A MINUTE"** message is displayed, the Main Selections Display for the Information Sub-system will appear as below:

```
**************************************
*                                    *
*        INFORMATION ACCESS          *
*                                    *
**************************************

1. DISPLAY - INFORMATION ON SPECIFIED CHEMICAL

2. ADD     - ADD NEW CHEMICAL

3. MODIFY  - ADD NEW PROPERTY

4. HELP    - HOW TO USE THIS PROGRAM

5. EXIT    - TO GAS SYSTEM MENU.

  SELECT ========>
```

To get into the DISPLAY ROUTINE, type 1 and press the RETURN key.

When this Main Selection Display is on the screen, any illegal commands entered by the user will cause a self-explanatory message to appear right beside the arrow. These error messages will disappear shortly so you may continue or try to enter another command.

3.3.2 Display Routine

The first 20 chemical names of the Synonym Table (see Appendix I) will be displayed.

```
1    ACETIC ACID
2    ACETIC ANHYDRIDE
3    ACETIC OXIDE
4    ACETONITRILE
5    ACRYLAMIDE
6    ACRYLIC ACID BUTYL ESTER
7    ACRYLIC AMIDE 50%
8    ACRYLONITRILE
9    ALBONE
10   ALUMINUM CHLORIDE
11   AMINOBENZENE
12   AMINOCAPROIC LACTAM
13   AMINOCYCLOHEXANE
14   2-AMINOETHANOL
15   BETA AMINOETHYL ALCOHOL
16   AMINOMETHANE
17   AMMONIA ANHYDROUS
18   AMMONIA WATER
19   AMMONIUM HYDROXIDE
20   N-AMYL ALCOHOL

  *** TYPE 'H' FOR HELP, 'E' TO EXIT ***

SELECT ========>
```

You might not see the chemical name that you want. Therefore, you need to "flip" the page back and forth. In order to see the next page, press the ⇓ key (no RETURN). And to see the previous page, press the ⇑ key (no RETURN).

If you want to "flip" more than 1 page at a time, keep the ⇓ (or ⇑) key pressed down until you want to stop and see where you are. Remember that the names (except those inserted at a later stage, see Section 3.3.4) are listed in alphabetical order. Typing 'H' at this point will produce helpful instructions.

When you have located the chemical name on the screen, type in the index number corresponding to that chemical. (This number is on the left side of the name.) Whatever you type in will appear on the screen to the right of "SELECT ⟹ " in the bottom line. If your chemical is UNLISTED, enter '267' as the index number.

After you type in the index number press the RETURN key. The information on the requested chemical will be displayed in the following format.

```
    ***  AMMONIA ANHYDROUS  ***

1   FORMULA              NH3
2   MOLECULAR WEIGHT     17.03
3   LATENT HEAT          1370            kJ/kg
4   BOILING POINT        -33             deg C
5   SOLUBILITY           89.9            g/100 ml
6   SPECIFIC GRAVITY     0.62(LIQ)
7   VAPOUR PRESSURE      76000(26 C      mm of Hg
8   VAPOUR DENSITY       0.6
9   FLASH POINT          NA
10  IDLH                 355             mg/m3
11  TLV                  18              mg/m3
12  STEL                 25              mg/m3
13  SP HEAT RATIO(VAP)   1.31
14  SYNONYMS
          1   AMMONIA ANHYDROUS
          2   LIQUID AMMONIA
15  FIRE HAZARD CODE (Press F for explanation)
          3      12

* PRESS 'U'NIT, 'C'HANGE, 'P'RINT, 'E'XIT, 'L'IST *
```

All the physical and chemical data are stored and presented in standard units as shown. The information access system will provide information in an alternative set of units (shown below) if requested by the user.

```
AMMONIA ANHYDROUS    NH3

MOLECULAR WEIGHT     17.03
LATENT HEAT          327          cal/g
BOILING POINT        -27.4        deg F
SOLUBILITY           89.9         g/100 ml
SPECIFIC GRAVITY     .62
VAPOUR PRESSURE      76000        mm of Hg
VAPOUR DENSITY       .6
FLASH POINT          NA
IDLH                 500          ppm
TLV                  25           ppm
STEL                 35           ppm
SP HEAT RATIO(VAP)   1.31
```

In some instances, terms such as "ND", "NF", and "NA" are used. "ND" means that the item could not be found in any of the sources searched. "NF" is used in the Flash Point field and means that the chemical is not flammable and therefore, no flash point. "NA" means that the field is not applicable for the displayed chemical.

The synonyms listed are considered to be the most common, and either the chemical name or the synonyms can be used for accessing the information stored in the system.

At this point, different options are available by pressing the appropriate letters:

'F' - to display the explanation of fire hazard codes (See Appendix II).

'U' - causes the information to be displayed in the alternative set of units (e.g. IDLH, TLV and STEL in ppm).

'C' - to enter the CHANGE ROUTINE (see below).

'P' - to print a hardcopy on a printer, if available.

'L' - to redisplay the list of chemical names so that another chemical can be selected.

'E' - to return to the Main Selection Display. Any illegal character will have the same effect.

3.3.3 Change Routine

As you enter the change routine, you will be asked to type in the password. Doing so correctly will display the list of physical and chemical properties, each accompanied by an item number and the appropriate unit. The system will also ask the item number of the property whose value you want to change. After typing in the number and pressing the RETURN key, the system will allow you to enter the new value of that property and ask whether you want to make more changes. A typical dialogue is shown on the next page.

You can change more than one item by doing so one at a time. When you respond 'N' to the 'More Changes?' question, the new information will be stored on the diskette and re-displayed on the screen.

```
PASS WORD:
    ***  AMMONIA ANHYDROUS  ***

 1  FORMULA
 2  MOLECULAR WEIGHT
 3  LATENT HEAT                          kJ/kg
 4  BOILING POINT                        deg C
 5  SOLUBILITY                           g/100 ml
 6  SPECIFIC GRAVITY
 7  VAPOUR PRESSURE                      mm of Hg
 8  VAPOUR DENSITY
 9  FLASH POINT                          deg C
 10 IDLH                                 ppm
 11 TLV                                  ppm
 12 STEL                                 ppm
 13 SP HEAT RATIO(VAP)
 14 SYNONYMS
 15 FIRE HAZARD CODE

CHOOSE NUMBER:? 1
 1 FORMULA : ? NH3
MORE CHANGES? Y OR N
```

3.3.4 Insert Routine

Entry to this routine requires a valid password. The system will first ask you to "ENTER NEW CHEMICAL NAME". Then it will repeatedly ask "ENTER SYNONYM - OR (RETURN) IF FINISHED" so that you can enter all the synonyms. After that, the system will establish a new record in the Information File and prompt you to enter values for the physical and chemical properties. Type in the corresponding data in the unit specified inside brackets in the prompt. When finished, the data will be written into the new record and stored on the diskette. The Main Selection Dispaly will then re-appear.

One drawback at this time is that the new chemical name and synonyms will only be appended to the end of the Synonym Table (See Appendix I), but not inserted in the proper alphabetical order. If you cannot locate a chemical name when you enter the DISPLAY ROUTINE, try checking the end of the chemical list to see whether a name has been inserted there at a later stage.

3.3.5 Modify Routine

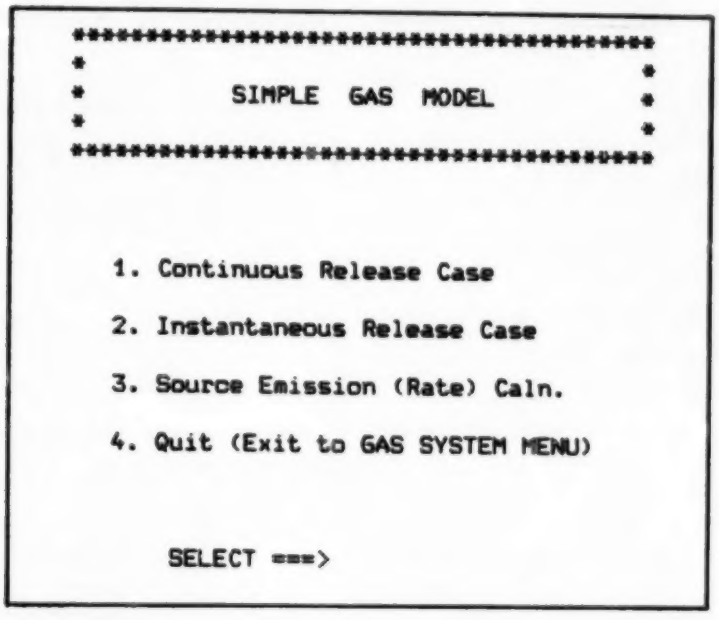
You also require a valid password to run this routine. After displaying a list of the existing properties with the default set of units, the system will ask "WHAT DO YOU WANT TO ADD?". Type in the property you want to include and the system will ask for its unit. The new list of properties will be

displayed after the modification has been recorded on the diskette. You can then use the DISPLAY ROUTINE to see that a blank space has been reserved for you to put in the value of the property newly included. Do so by invoking the CHANGE ROUTINE (Section 3.3.3).

3.4 SIMPLE GAS MODEL

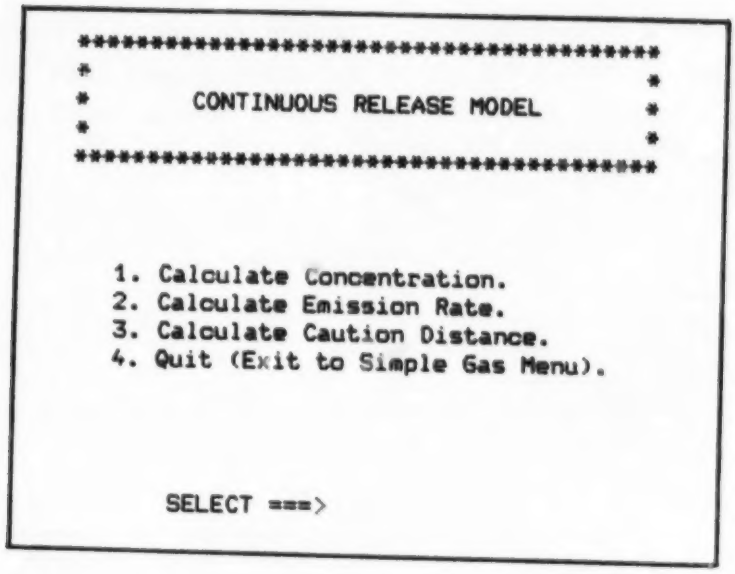
3.4.1 Selection Phase

The Simple Gas Model Menu below allows you to choose between calculations for the Continuous Release (Plume) Case, the Instantaneous Release (Puff) Case or Source Strength.


SIMPLE GAS MODEL
1. Continuous Release Case
2. Instantaneous Release Case
3. Source Emission (Rate) Caln.
4. Quit (Exit to GAS SYSTEM MENU)
SELECT ===>

This program is highly user-friendly and step-by-step menus or instructions are displayed on the screen. The following is an example for the concentration calculations in the Continuous Release Case. The first step is to type '1' and press the RETURN key from this main menu to choose the Continuous Release Case calculation. Make another choice if you want to run another routine. Then follow displayed instructions which guide you along in your calculations.

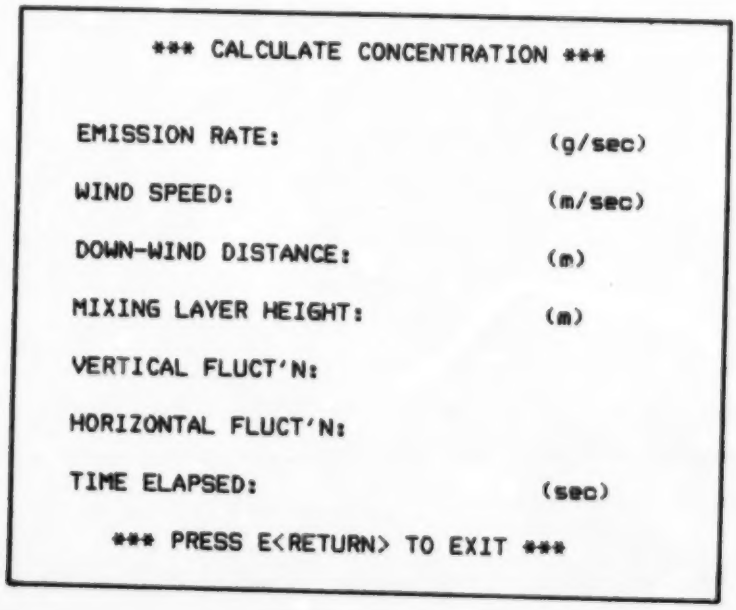
The next menu will allow you to select different routines as shown below:



To get into a routine, type the routine number followed by the RETURN key. For example, if you want to calculate the concentration, type 1 and press (RETURN).

3.4.2 Input Phase

Each selection command will cause the appropriate input panel to be displayed in the format below:



If you have the input in units other than those displayed, repeatedly press 'U' and (RETURN) until the unit you want is displayed. Now, enter the data.

Default values are available for some of the entries, i.e. if you do not know the right value, the computer will insert a reasonable value. You can use the default value by simply pressing (RETURN) without typing in any value, or by typing D or DEFAULT followed by (RETURN). If no default value is available, you will hear a beep and you must supply a value.

If you want to change any input already entered, type 'C' and (RETURN). Then a new input panel with blank entries will be displayed. But all the input you have entered up to this point has been saved, and can be retrieved if necessary.

You can recall the previous values of any desired entry (values you entered before) by simply pressing (RETURN). For the entry that needs changing, just type in a new value followed by (RETURN). This feature is useful when you want to calculate the concentration (or emission, etc.) more than once with the same set of inputs, except for one input entry that keeps changing. For example, if you want to know concentrations at different distances from the source of gas release, you will use the same set of inputs, except for the down wind distance.

If you make a typing error, you can press the left arrow (⇐) to erase the last character or the '@' key (SHIFT-2) to erase the current entry.

Help messages pertaining to various inputs are available. You can get at them by typing 'H' and (RETURN) at the appropriate input.

Typing 'E' and (RETURN) when an input panel is displayed will get you back to the previous menu. Then you can choose another calculation, e.g. for Caution Distance.

An example of the filled input panel for a concentration calculation is shown below. Note that the unit for emission rate has been changed from (g/sec) to (kg/sec) using the 'U' command.

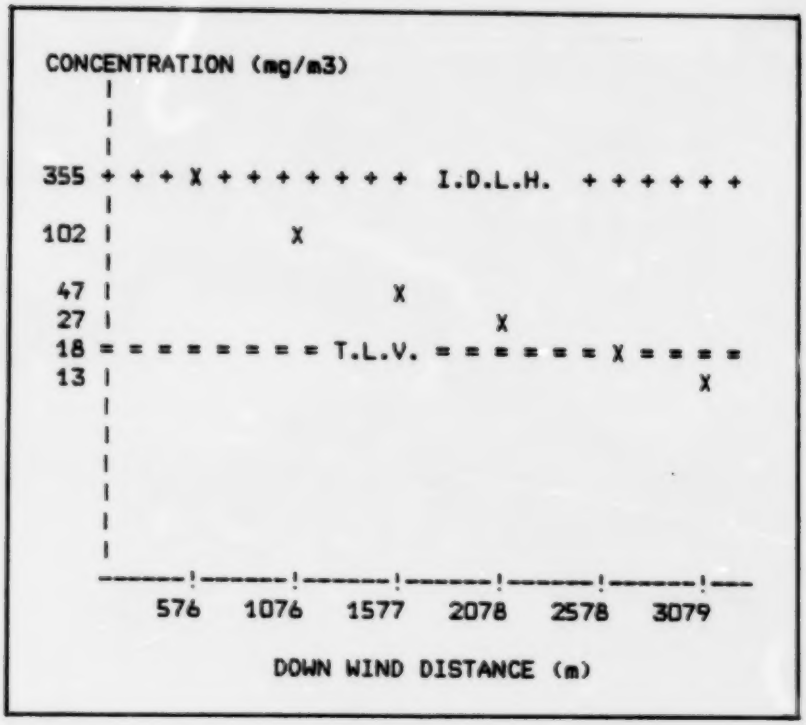
```
      *** CALCULATE CONCENTRATION ***

EMISSION RATE:          20          (kg/sec)
WIND SPEED:             5           (m/sec)
DOWN-WIND DISTANCE:     5000        (m)
MIXING LAYER HEIGHT:    300         (m)
VERTICAL FLUCT'N:       0.1
HORIZONTAL FLUCT'N:     0.17
TIME ELAPSED:           3600        (sec)
  *** PRESS ANY KEY TO CONTINUE ***
```

3.4.3 Output Phase

The answer is given in two different units as shown below. To put this concentration into perspective, the IDLH, STEL and TLV values are also quoted in (mg/m^3).

```
**************
CONCENTRATION
**************


7.84314             (mg/m3)
4.89688E-07         (lb./ft3)

*** IDLH:  354.8    (mg/m3) ***
*** STEL:  24.8     (mg/m3) ***
*** TLV:   17.7     (mg/m3) ***


****************
PLUME FULL-WIDTH
****************

1700                (m)
5577.7              (ft)


*** PRESS 'G' FOR GRAPHICS, 'E' TO EXIT ***
```

At this point, a graphic display of concentration against distance can be obtained by pressing 'G'. Note that the concentration scale is logarithmic. The IDLH and TLV levels are also drawn. The IDLH and TLV distances can be easily read from the graph.



Hard copies of this graph can be obtained by pressing 'P' if a printer is available.

3.4.4 Summary of Valid Entries for the Simple Gas Model

Numeric (RETURN)

- any valid MBASIC signed or unsigned integer, real or double precision number

  e.g. 1.3
  -3
  2.5E-3
  -.1
  1D2

- any character(s) following and including the first invalid character will be ignored.

H or HELP (RETURN)

- to display help messages.

U or UNIT (RETURN)

- to change unit in Simple Gas Model.

C or CLEAR (RETURN)

- to clear all input fields.

D or DEFAULT or (null) (RETURN)

- to use default value.

E or EXIT (RETURN)

- to get back to the previous menu.

⇐ (left arrow)

- erase one character and move the cursor one position to left.

@ (shift-2)

- erase current field.

3.5 HEAVY GAS MODEL

3.5.1 Input Phase

This model requires the input of 14 parameters. Most of them have default values. These are listed at the beginning of the run. Questions are then presented sequentially as input panels, so that you can supply or change the parameters. Typical input panels are shown below:

```
[Q6]     Weight of the Gas Released




-------------------------------------------------------------

  ENTER YOUR INPUT HERE ===>                          (kg)

-------------------------------------------------------------

    ENTER    value
             Qn     to jump to Question n
             L      to List all parameters
             <rtn>  to use default value
             R      to Run the model
             E      to Exit
```

```
[Q14]    Mean Wind Speed

         Very Strong wind:  10 m/sec
         Strong wind      :   7 m/sec
         Average wind     :   5 m/sec  DEFAULT VALUE
         Mild wind        :   3 m/sec
         Very mild wind   :   1 m/sec
         * Do NOT use wind speed < .1 m/sec

-------------------------------------------------------------

  ENTER YOUR INPUT HERE ===>                        (m/sec)

-------------------------------------------------------------

    ENTER    value
             Qn     to jump to Question n
             L      to List all parameters
             <rtn>  to use default value
             R      to Run the model
             E      to Exit
```

The middle area is for receiving input. The upper area displays the default value, if available, and other helpful information. Valid input commands are listed in the bottom. By typing 'Qn (RETURN)', when n is an integer from 1 to 14, you can jump directly to Question Qn. Typing 'L (RETURN)' will produce a list of the input parameters. Typing 'R (RETURN)' or 'E (RETURN)' respectively will execute or terminate the model. If you want to use the default value, just press (RETURN). There is no default value for the amount of gas released (Question Q6). The model will not run unless this parameter is supplied.

A typical list of parameters, which will also appear automatically after you answer Question Q14, is as follows:

```
-------------------------------------------------
     L I S T   O F   P A R A M E T E R S
-------------------------------------------------

***** DEFAULT CHEMICAL : NH3 *****

   [Q 1 ]  Molecular Weight  17.03
   [Q 2 ]  Boiling Point     -33       (deg C)
   [Q 3 ]  Latent Heat, Gas  1370      (kJ/kg)
   [Q 4 ]  Initial Radius    45        (m)
   [Q 5 ]  Latent Heat, Wat  2260      (kJ/kg)
   [Q 6 ]  Release Amount    20000     (kg)
   [Q 7 ]  Gas in Liquid     0.8
   [Q 8 ]  Ambient Temp.     20        (deg C)
   [Q 9 ]  Vert. Entr. Coef. 0.4
   [Q 10 ]  Mixing Layer Ht. 300       (m)
   [Q 11 ]  Water Vapour     0.01
   [Q 12 ]  Ambient Pressure 1.0       (atm)
   [Q 13 ]  Friot. to Mean   0.17
   [Q 14 ]  Wind Speed       3         (m/sec)
```

You can request a hardcopy by pressing 'P'.

3.5.2 Execution Phase

You enter the execution phase by entering 'R' when an input panel is displayed. The system will ask "INTERMEDIATE RESULTS NEEDED?". Responding with 'Y (RETURN)' will result in a series of displays of the intermediate results such as the mass of air entrained, volume, initial height and density of cloud, and end of slumping phase information. You also have the option to override some of these by answering with 'Y (RETURN)' when prompted.

Armed with these intermediate results, the system will go on to calculate the cloud characteristics as a function of downwind distance. You will be asked to enter the range and the increment in distance that you want the calculation done. The result is a table, which can either be displayed on screen, or printed if a printer is available, as follows:

* CLOUD CHARACTERISTICS *

DIST. (m)	PASSING-TIME(sec) Cntr	Head	Tail	CONC'N. (mg/m3)	RADIUS (m)	HEIGHT (m)
0	0	0	36	90948	45	34.6
50	17	2	80	90948	112	5.6
100	33	18	112	90948	152	3.0
150	50	35	140	90948	183	2.1
200	67	52	166	90948	210	1.6
250	83	59	191	90948	234	1.3
300	100	64	215	90948	255	1.1
350	117	72	239	90948	275	0.9
400	133	81	262	90948	294	0.8
450	150	91	271	65283	311	1.0
500	167	101	292	13414	328	4.4
550	183	112	312	6845	345	7.8
600	200	124	333	4331	362	11.2
650	217	136	353	3032	379	14.6
700	233	148	373	2253	396	18.0
750	250	160	394	1742	413	21.4
800	267	172	414	1387	430	24.8
850	283	185	435	1129	447	28.2
900	300	198	455	935	464	31.6
950	317	212	476	786	481	35.0
1000	333	227	496	668	498	38.4
1050	350	242	517	574	515	41.8
1100	367	257	537	497	532	45.2
1150	383	271	558	434	549	48.6
1200	400	286	578	382	566	52.0
1250	417	301	599	338	583	55.4
1300	433	316	619	301	600	58.8
1350	450	330	639	269	617	62.2
1400	467	345	660	241	634	65.6
1450	483	360	680	218	651	69.0
1500	500	375	701	197	668	72.4
1550	517	390	721	179	685	75.8
1600	533	404	742	163	702	79.2
1650	550	419	762	149	719	82.6
1700	567	434	783	137	736	86.0
1750	583	449	803	126	753	89.4
1800	600	464	824	116	770	92.8
1850	617	478	844	107	787	96.2
1900	633	493	865	99	804	99.6
1950	650	508	885	92	821	103.0
2000	667	523	905	85	838	106.4

This table of cloud characteristics gives, for each downwind distance, the time required for the centre, the head and the tail of the cloud to pass through that point. The difference of the latter two times gives the time of exposure. It also gives the concentration at the cloud centre, the radius and height of the cloud when the cloud is centred at that particular distance. For comparison, the IDLH, STEL and TLV values are displayed on the screen.

Figure 5 is a graph of concentration against downwind distance predicted by both the Heavy Gas Model and the Simple Gas Model for an instantaneous release of 20,000 kg of ammonia. The agreement between the two models is pretty good. During the slumping phase, the concentration predicted by the Heavy Gas Model remains at a constant high value. This is more realistic than the Simple Gas Model, which predicts infinite concentration at zero distance. A plot of the height of the cloud versus time is shown in Figure 6. The height decreases rapidly at the beginning. It levels off to a minimum at the end of the slumping phase and then increases again when atmospheric turbulence dominates. This figure agrees reasonably well with Figure 3 in Kaiser and Walker's paper, which gives a plot of the height as a function of time, using a more "complete" model.

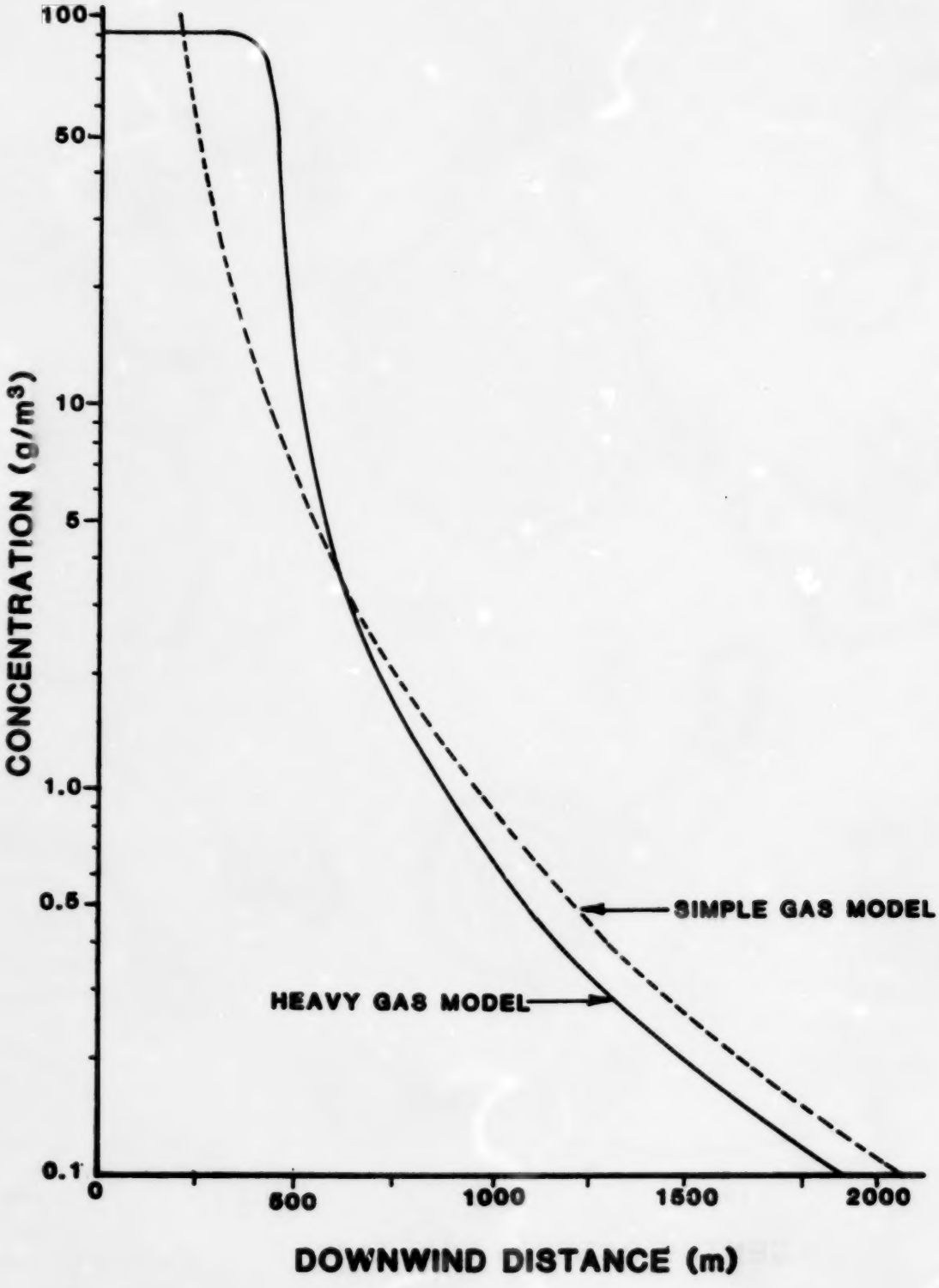

100
50
10
5
1.0
0.5
0.1
CONCENTRATION (g/m³)
0
500
1000
1500
2000
DOWNWIND DISTANCE (m)
SIMPLE GAS MODEL
HEAVY GAS MODEL

Figure 5

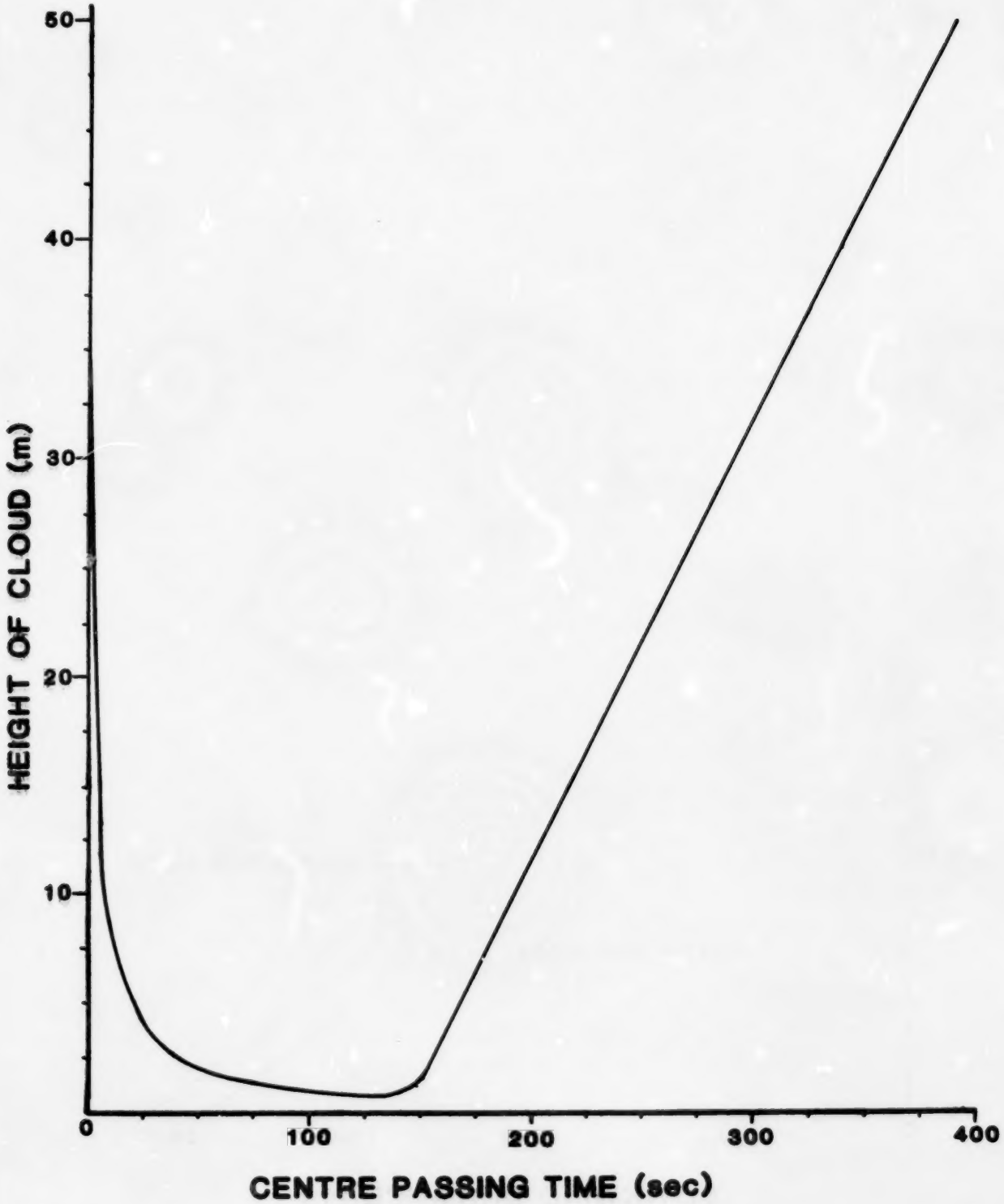

50
40
30
20
10
HEIGHT OF CLOUD (m)
0
100
200
300
400
CENTRE PASSING TIME (sec)

Figure 6

3.5.3 Summary of Valid Entries for the Heavy Gas Model

During the input phase you may enter

a number

- any number in the form acceptable by MBASIC syntax.

  e.g. 1.1234
  -123.09
  .023
  3.5D2
  7E-3
  -.234E-21

Qn

- where n is an integer between 1 and 14, to bring you Question n.

L

- to list all the parameters with input or default values. Then you can press 'P' to get a hardcopy. Note that some physical properties are taken directly from the information access program. The chemical last accessed when you run the INFORMATION ACCESS program is used as default.

R

- to execute the model.

E

- to terminate the model and return to GAS SYSTEM MENU.

CHAPTER 4: PROGRAMS

4.0 PROGRAMS

4.1 SYSTEM DESIGN AND FLOW CHARTS

This portable computing system for use in toxic gas emergencies (the GAS SYSTEM) was developed for use in an Osborne 1 portable computer, with either single or double density disk drives. It requires 64 K of random access memory and two floppy-disk drives. The programs are interactively written in Microsoft Basic (MBASIC) using the CP/M operating system. Programs and files are stored in two 5¼ inch single-density diskettes (92 K each) along with the MBASIC interpreter and some CP/M utility program modules.

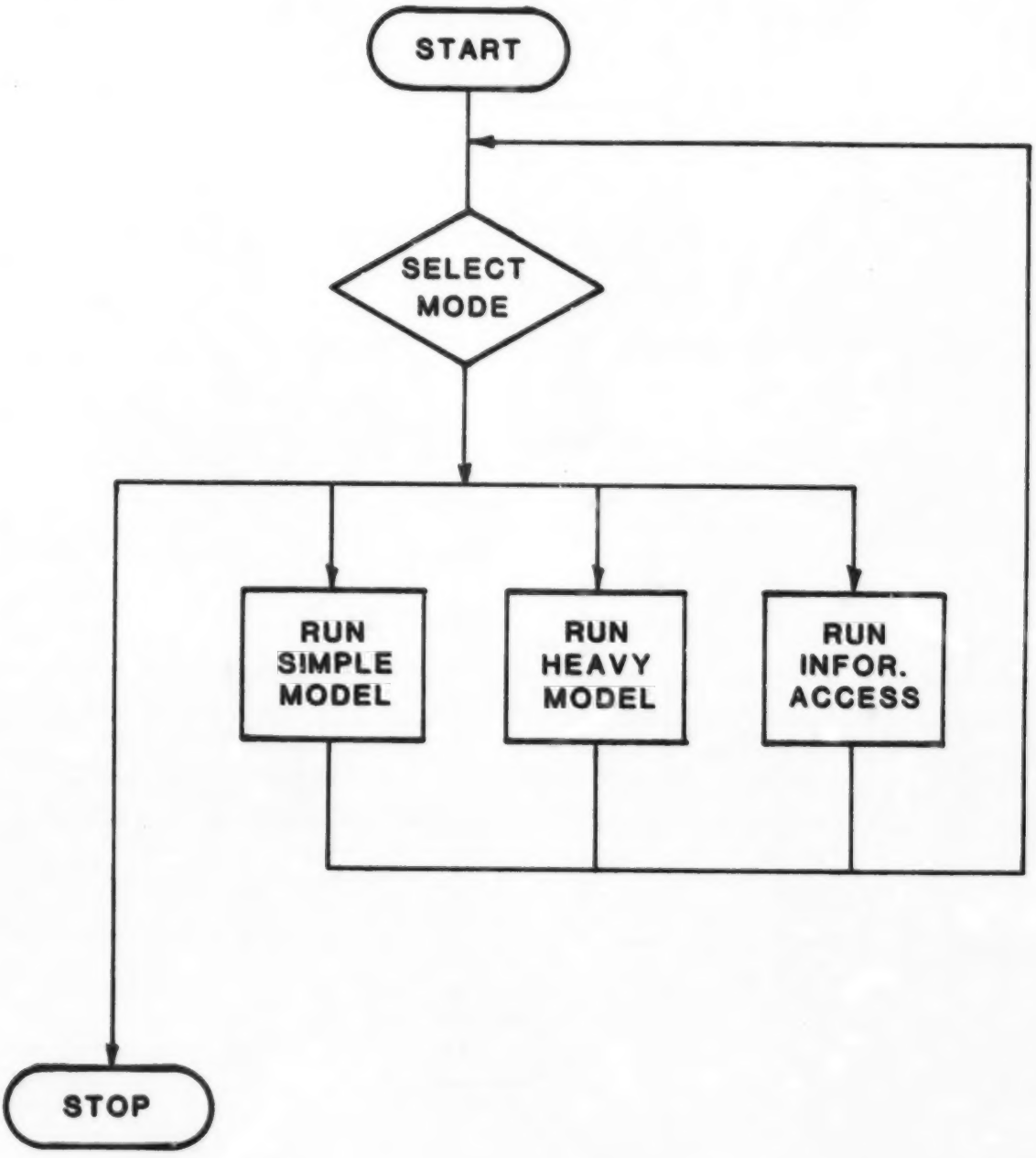
The GAS SYSTEM is menu-driven and consists of the following three main programs:

1) A: SIMPLE2 - the Simple Gas Model
2) A: HEAVY - the Heavy Gas Model
3) B: INFO2 - the Information Sub-System

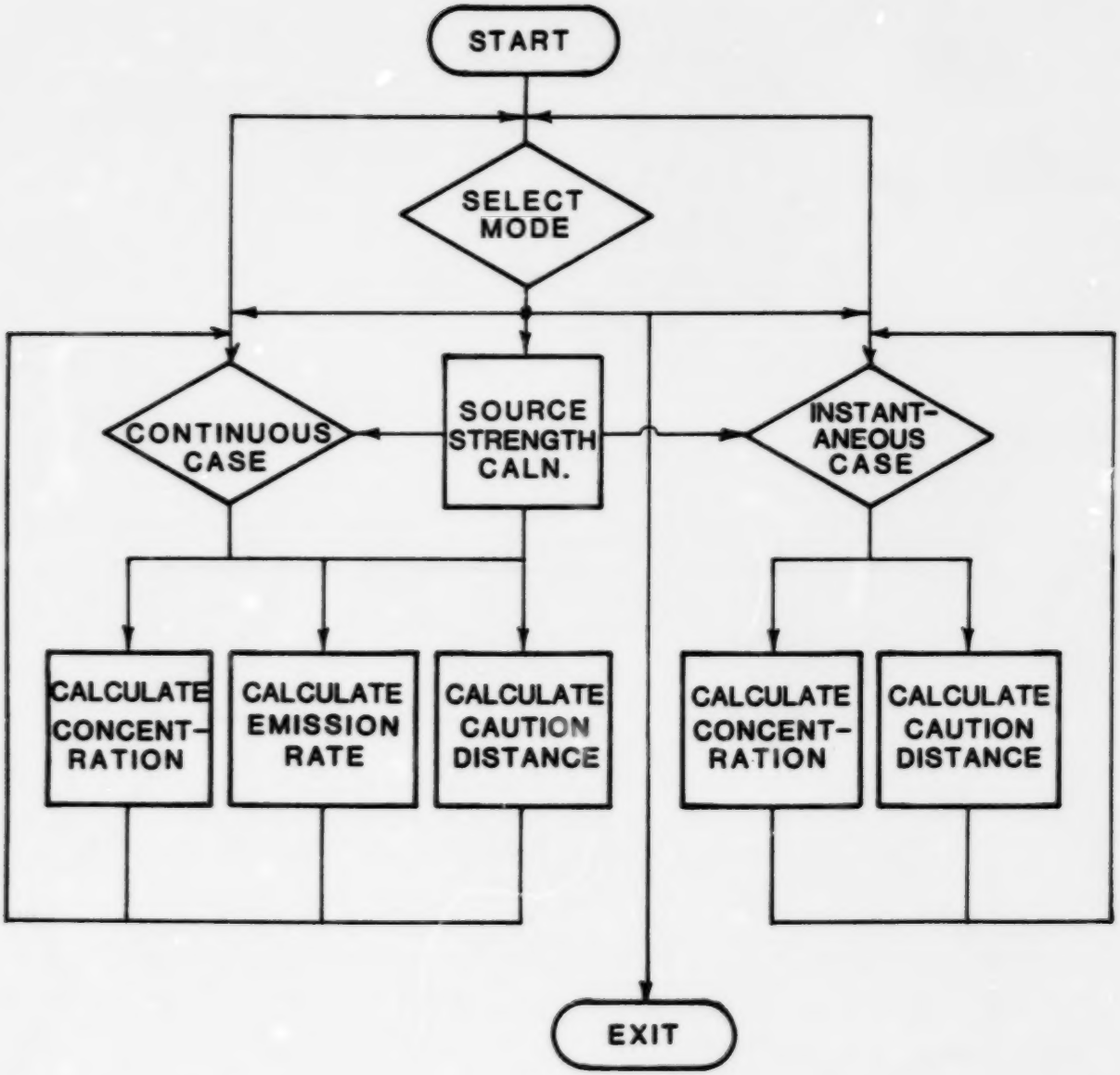
Here A: and B: refer to the diskette on which the programs reside: A: is usually put into the disk drive on the left-hand side of the Osborne 1 computer.

Flow charts on the following pages outline the functions of various programs and routines, as well as their inter-relationship. More detailed description is given in the User's Manual (Chapter 3).

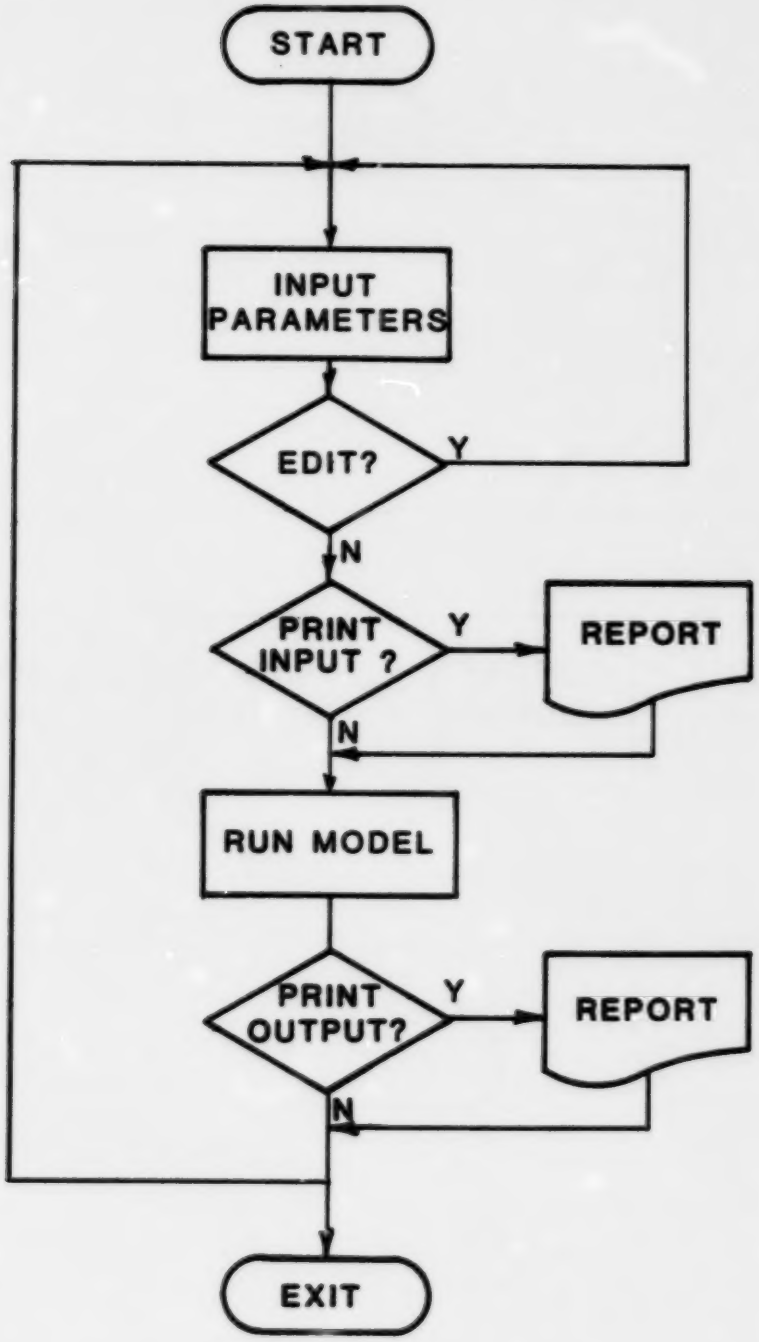
GAS SYSTEM


START
SELECT MODE
RUN SIMPLE MODEL
RUN HEAVY MODEL
RUN INFOR. ACCESS
STOP

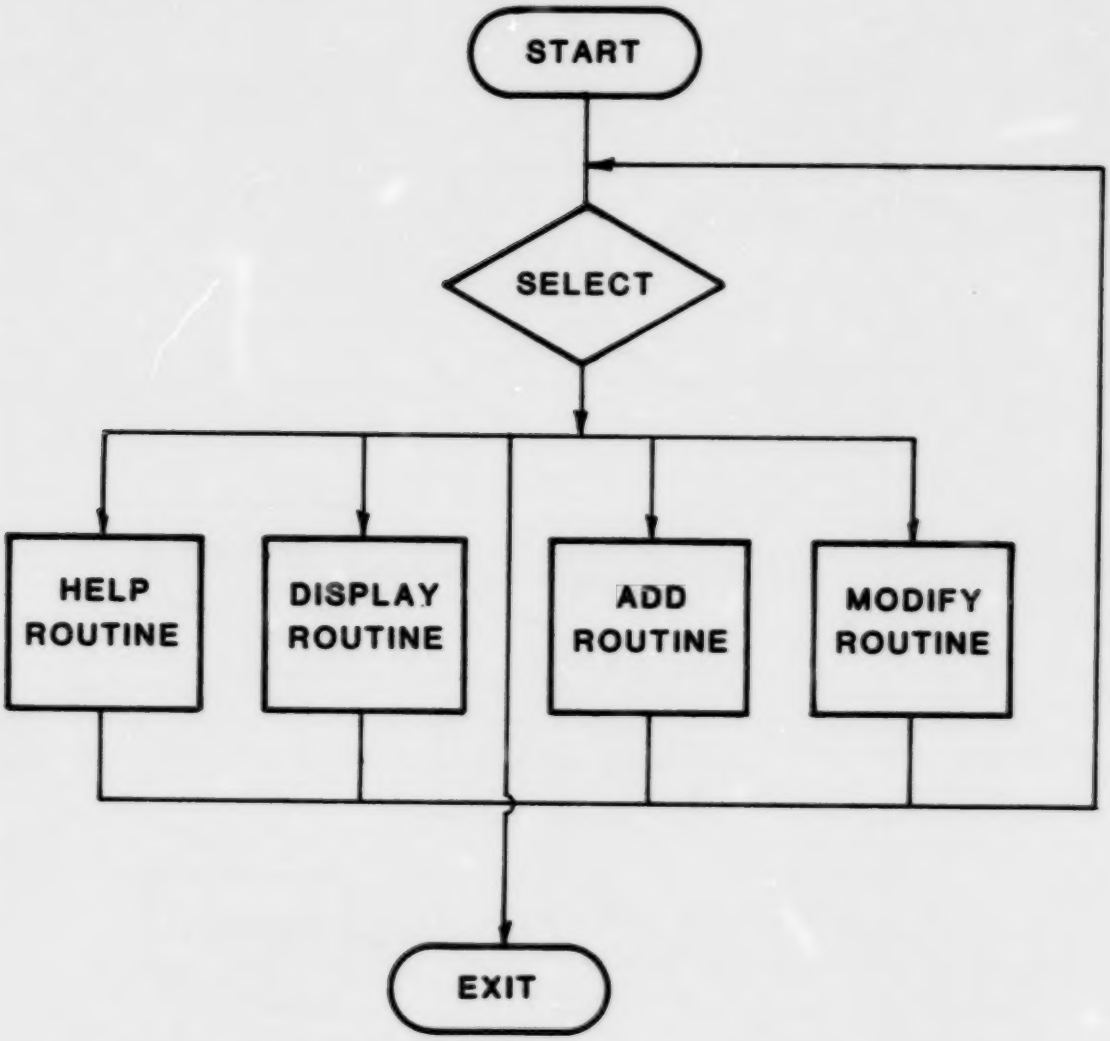
SIMPLE GAS MODEL



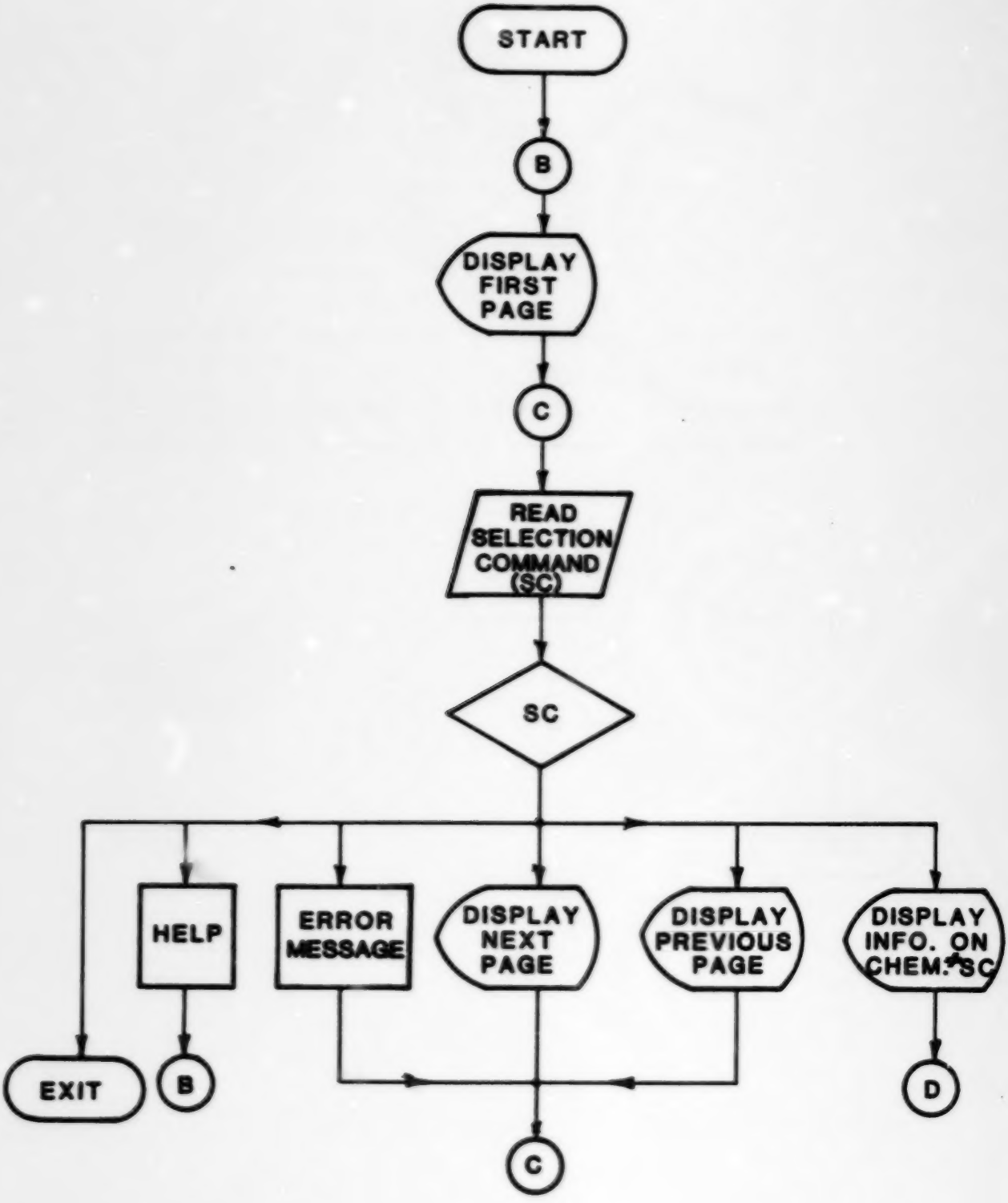
HEAVY GAS MODEL



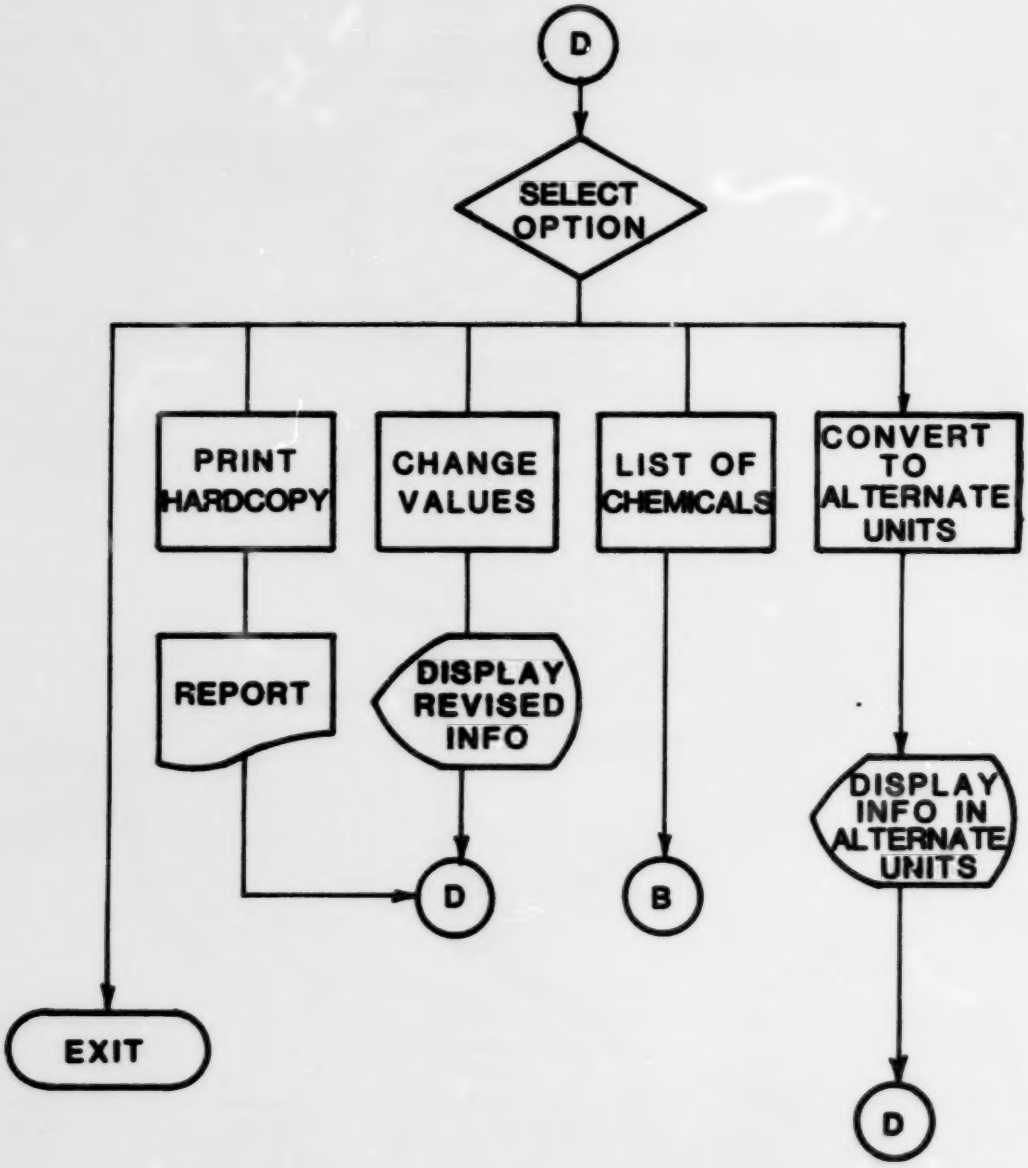
INFORMATION SUBSYSTEM



DISPLAY ROUTINE



DISPLAY ROUTINE (CONT.)



4.2 FILE STRUCTURES FOR INFORMATION SUB-SYSTEM

4.2.1 Information File

This is actually made up by joining two random access files, B:INFO.RAF and B:INF2.RAF on disk B:. The resulting file structure has an effective record length of 237 characters distributed among 26 fields as follows:

FIELD	FIELD NAME	LENGTH
1	Chemical Formula	16
2	Molecular Weight	10
3	Latent Heat	
4	Boiling Point	
5	Solubility	16
6	Specific Gravity	10
7	Vapour Pressure	
8	Vapour Density	
9	Flash Point	
10	IDLH	
11	TLV	
12	STEL	
13	Specific Heat Ratio	
14-21	for future expansion	10 each
22-26	Fire Hazard Code	3 each

Presently, there are 79 records, each containing information on one chemical. Future expansion to include more chemicals is only limited by the capacity of the disk. The 79 current chemicals, arranged in alphabetical order, are assigned consecutive record numbers. These are used by the program to retrieve the record containing the information on the respective chemicals.

4.2.2 Chemical Name File

Most of the 79 chemicals have more than one name (synonyms). These 266 chemical names are stored in a sequential file B:CHEM.NAM. Each name is paired up with the record number used to retrieve the appropriate record from the Information File. The program will load the content of this file into two tables with a common index:

Synonym Table (array STN$) - containing the synonyms.

Synonym Table Link (array STL) - containing the record numbers.

4.2.3 Synonym File

This sequential file, named B:SYNO.NAM, contains 79 groups of numerical indices delimited by zeros. Each group contains all the indices to retrieve the synonyms of a particular chemical from the Synonym Table (array STN$).

4.2.4 Parameters File

The contents of this sequential file B:PARA.NAM are labels of the physical and chemical properties (i.e. field names of the Information File) and their associated units.

APPENDIX

I. SYNONYM TABLE

INDEX	SYNONYM	CHEMICAL NAME
1.	ACETIC ACID	ACETIC ACID
2.	ACETIC ANHYDRIDE	ACETIC ANHYDRIDE
3.	ACETIC OXIDE	ACETIC ANHYDRIDE
4.	ACETONITRILE	ACETONITRILE
5.	ACRYLAMIDE	ACRYLAMIDE
6.	ACRYLIC ACID, BUTYL ESTER	N-BUTYL ACRYLATE
7.	ACRYLIC AMIDE 50%	ACRYLAMIDE
8.	ACRYLONITRILE	ACRYLONITRILE
9.	ALBONE	HYDROGEN PEROXIDE
10.	ALUMINUM CHLORIDE	ALUMINUM CHLORIDE
11.	AMINOBENZENE	ANILINE
12.	AMINOCAPROIC LACTAM	CAPROLACTAM
13.	AMINOCYCLOHEXANE	CYCLOHEXYLAMINE
14.	2-AMINOETHANOL	MONOETHANOLAMINE
15.	beta-AMINOETHYL ALCOHOL	MONOETHANOLAMINE
16.	AMINOMETHANE	METHYLAMINE
17.	AMMONIA ANHYDROUS	AMMONIA ANHYDROUS
18.	AMMONIA WATER	AMMONIA HYDROXIDE
19.	AMMONIUM HYDROXIDE	AMMONIUM HYDROXIDE
20.	n-AMYL ALCOHOL	n-AMYL ALCOHOL
21.	1-AMYL ALCOHOL	n-AMYL ALOCHOL
22.	ANHYDROUS ALUMINUM CHLORIDE	ALUMINUM CHLORIDE
23.	ANILINE	ANILINE
24.	ANILINE OIL	ANILINE
25.	ANILINOBENZENE	DIPHENYLAMINE
26.	AQUA FORTIS	NITRIC ACID
27.	AQUEOUS AMMONIA	AMMONIUM HYDROXIDE
28.	AROCLOR	POLYCHLORINATED BIPHENYL
29.	ASKAREL	POLYCHLORINATED BIPHENYL
30.	AZOTIC ACID	NITRIC ACID

INDEX	SYNONYM	CHEMICAL NAME
31.	BATTERY ACID	SULPHURIC ACID
32.	BENZENE	BENZENE
33.	BENZOL	BENZENE
34.	BENZOLE	BENZENE
35.	BLUE OIL	ANILINE
36.	BROMINE	BROMINE
37.	BUTYL ACRYLATE	n-BUTYL ACRYLATE
38.	n-BUTYL ACRYLATE	n-BUTYL ACRYLATE
39.	n-BUTYLCARBINOL	n-AMYL ALCOHOL
40.	n-BUTYL 2-PROPENOATE	n-BUTYL ACRYLATE
41.	CALCIUM OXIDE	CALCIUM OXIDE
42.	CALX	CALCIUM OXIDE
43.	CAPROLACTAM	CAPROLACTAM
44.	CARBOLIC ACID	PHENOL
45.	CARBON BISULFIDE	CARBON DISULFIDE
46.	CARBON DISULFIDE	CARBON DISULFIDE
47.	CARBON TET	CARBON TETRACHLORIDE
48.	CARBON TETRACHLORIDE	CARBON TETRACHLORIDE
49.	CHLORINATED BIPHENYL	POLYCHLORINATED BIPHENYL
50.	CHLORINE	CHLORINE
51.	1-CHLORO-2, 3-EPOXYPROPANE	EPICHLOROHYDRIN
52.	CHLOROETHANE	ETHYL CHLORIDE
53.	CHLOROETHENE	VINYL CHLORIDE
54.	CHLOROETHYLENE	VINYL CHLORIDE
55.	CHLOROFORM	CHLOROFORM
56.	CHLOROMETHANE	METHYL CHLORIDE
57.	gamma-CHLOROPROPYLENE OXIDE	EPICHLOROHYDRIN
58.	CHLOROSULPHONIC ACID	CHLOROSULPHONIC ACID
59.	CHLORSULPHONIC ACID	CHLOROSULPHONIC ACID
60.	CRESOLS	CRESOLS
61.	CRESYLIC ACID	CRESOLS
62.	CYANOGRAN	SODIUM CYANIDE
63.	CYANOETHYLENE	ACRYLONITRILE
64.	CYANOMETHANE	ACETONITRILE
65.	CYCLOHEXYLAMINE	CYCLOHEXYLAMINE

INDEX	SYNONYM	CHEMICAL NAME
66.	2,4-D	2,4-DICHLOROPHENOXYACETIC ACID
67.	1,6-DIAMINOHEXANE	HEXAMETHYLENEDIAMINE
68.	1,2-DIBROMOETHANE	ETHYLENE DIBROMIDE
69.	DICHLORIDE	1,4-DICHLOROBENZENE
70.	1,4-DICHLOROBENZENE	1,4-DICHLOROBENZENE
71.	p-DICHLOROBENZENE	1,4-DICHLOROBENZENE
72.	1,2-DICHLOROETHANE	ETHYLENE DICHLORIDE
73.	DICHLOROMETHANE	DICHLOROMETHANE
74.	2,4-DICHLOROPHENOXYACETIC ACID	DICHLOROPHENOXYACETIC ACID
75.	DIETHYLENEIMIDE OXIDE	MORPHOLINE
76.	DIISOBUTYLENE	DIISOBUTYLENE
77.	DIPHENYLAMINE	DIPHENYLAMINE
78.	DIPHENYLMETHANEDIISOCYANATE	DIPHENYLMETHANEDIISOCYANATE
79.	DIPHENYLMETHANE-4, 4-DIISOCYANATE	DIPHENYLMETHANEDIISOCYANATE
80.	DOWICIDE	PENTACHLOROPHENOL
81.	EB	ETHYLBENZENE
82.	EDB	ETHYLENE DIBROMIDE
83.	EDC	ETHYLENE DICHLORIDE
84.	ELEMENTAL PHOSPHORUS	PHOSPHORUS
85.	EPICHLOROHYDRIN	EPICHLOROHYDRIN
86.	1,2-EPOXYETHANE	ETHYLENE OXIDE
87.	1,2-EPOXYPROPANE	PROPYLENE OXIDE
88.	ETHANEDIOIC ACID	OXALIC ACID
89.	ETHANENITRILE	ACETONITRILE
90.	ETHANOIC ACID	ACETIC ACID
91.	ETHANOIC ANHYDRIDE	ACETIC ANHYDRIDE
92.	ETHANOLAMINE	MONOETHANOLAMINE
93.	ETHER HYDROCHLORIC	ETHYL CHLORIDE
94.	ETHYLBENZENE	ETHYLBENZENE
95.	ETHYLBENZOL	ETHYLBENZENE
96.	ETHYLCARBINOL	n-PROPYL ALCOHOL
97.	ETHYL CHLORIDE	ETHYL CHLORIDE
98.	ETHYLENE BROMIDE	ETHYLENE DIBROMIDE
99.	ETHYLENE CHLORIDE	ETHYLENE DICHLORIDE
100.	ETHYLENE DIBROMIDE	ETHYLENE DIBROMIDE

INDEX	SYNONYM	CHEMICAL NAME
101	ETHYLENE DICHLORIDE	ETHYLENE DICHLORIDE
102.	ETHYLENE OXIDE	ETHYLENE OXIDE
103.	ETHYLENE TETRACHLORIDE	PERCHLOROETHYLENE
104.	ETHYLENE TRICHLORIDE	TRICHLOROETHYLENE
105.	FERTILIZER ACID	SULPHURIC ACID
106.	FLUORHYDRIC ACID	HYDROFLUORIC ACID
107.	FORMALDEHYDE	FORMALDEHYDE
108.	FORMALDEHYDE POLYMER	PARAFORMALDEHYDE
109.	FORMALIN	FORMALDEHYDE
110.	FORMALIN	FORMALDEHYDE
111.	FORMIC ACID	FORMIC ACID
112.	FORMIC ALDEHYDE	FORMALDEHYDE
113.	FORMYLIC ACID	FORMIC ACID
114.	2-FURANCARBINOL	FURFURYL ALCOHOL
115.	2,5-FURANEDIONE	MALEIC ANHYDRIDE
116.	FURFURALCOHOL	FURFURYL ALCOHOL
117.	FURFURYL ALCOHOL	FURFURYL ALCOHOL
118.	2-FURYL-METHANOL	FURFURYL ALCOHOL
119.	FYDE	FORMALDEHYDE
120.	GLACIAL ACETIC ACID	ACETIC ACID
121.	HEXAHYDROANILINE	CYCLOHEXYLAMINE
122.	HEXAMETHYLENEDIAMINE	HEXAMETHYLENEDIAMINE
123.	1,6-HEXANEDIAMINE	HEXAMETHYLENEDIAMINE
124.	HYDROCHLORIC ACID	HYDROCHLORIC ACID
125.	HYDROCHLORIC ACID ANHYDROUS	HYDROGEN CHLORIDE ANHYDROUS
126.	HYDROCYANIC ACID SODIUM SALT	SODIUM CYANIDE
127.	HYDROFLUORIC ACID	HYDROFLUORIC ACID
128.	HYDROFLUORIC ACID ANHYDROUS	HYDROGEN FLUORIDE
129.	HYDROFLUORIC ACID AQUEOUS	HYDROFLUORIC ACID
130.	HYDROGEN CHLORIDE ANHYDROUS	HYDROGEN CHLORIDE
131.	HYDROGEN DIOXIDE	HYDROGEN PEROXIDE
132.	HYDROGEN FLUORIDE	HYDROGEN FLUORIDE
133.	HYDROGEN PEROXIDE	HYDROGEN PEROXIDE
134.	HYDROGEN SULFIDE	HDYROGEN SULFIDE
135.	HYDROXYBENZENE	PHENOL

INDEX	SYNONYM	CHEMICAL NAME
136.	2-HYDROXYETHYLAMINE	MONOETHANOLAMINE
137.	2-HYDROXYMETHYLFURAN	FURFURYL ALCOHOL
138.	HYDROXYTOLUENES	CRESOLS
139.	HYLENE T	TOLUENE-2,4-DIISOCYANATE
140.	LEAD TETRAETHYL	TETRAETHYL LEAD
141.	LEAD TETRAMETHYL	TETRAMETHYL LEAD
142.	LIQUID AMMONIA	AMMONIA ANHYDROUS
143.	MALEIC ANHYDRIDE	MALEIC ANHYDRIDE
144.	MDI	DIPHENYLMETHANEDIISOCYANATE
145.	MERCURIALIN	METHYLAMINE
146.	METHANAL	FORMALDEHYDE
147.	METHANOIC ACID	FORMIC ACID
148.	METHYLAMINE	METHYLAMINE
149.	METHYLBENZENE	TOLUENE
150.	METHYLBENZOL	TOLUENE
151.	METHYL CHLORIDE	METHYL CHLORIDE
152.	METHYL CHLOROFORM	1,1,1-TRICHLOROETHANE
153.	METHYL CYANIDE	ACETONITRILE
154.	METHYLENE CHLORIDE	DICHLOROMETHANE
155.	METHYLENE DICHLORIDE	DICHLOROMETHANE
156.	METHYLENE OXIDE	FORMALDEHYDE
157.	METHYL OXIRANE	PROPYLENE OXIDE
158.	METHYLPHENOLS	CRESOLS
159.	MIXTURE OF BENZENE, TOLUENE AND XYLENES	NAPTHTHA (COAL TAR)
160.	MONDUR TDS	TOLUENE-2,4-DIISOCYANATE
161.	MONOETHANOLAMINE	MONOETHANOLAMINE
162.	MONOMETHYLAMINE	METHYLAMINE
163.	MORPHOLINE	MORPHOLINE
164.	MURIATIC ACID	HYDROCHLORIC ACID
165.	NACCONATE 100	TOLUENE-2,4-DIISOCYANATE
166.	NAPHTHA (COAL TAR)	NAPHTHA (COAL TAR)
167.	NAPHTHALENE	NAPHTHALENE
168.	NAPHTHALINE	NAPHTHALENE
169.	NITRIC ACID	NITRIC ACID
170.	OIL OF VITRIOL	SULPHURIC ACID

INDEX	SYNONYM	CHEMICAL NAME
171.	2-OXOHEXAMETHYLENIMINE	CAPROLACTAM
172.	ORTHOPHOSPHORIC ACID	PHOSPHORIC ACID
173.	OXALIC ACID	OXALIC ACID
174.	OXIRANE	ETHYLENE OXIDE
175.	OXYTOLUENES	CRESOLS
176.	PARADI	p-DICHLOROBENZENE
177.	PARADICHLOROBENZENE	p-DICHLOROBENZENE
178.	PARADOW	p-DICHLOROBENZENE
179.	PARAFORM	PARAFORMALDEHYDE
180.	PARAFORMALDEHYDE	PARAFORMALDEHYDE
181.	PCB	POLYCHLORINATED BIPHENYL
182.	PCP	PENTACHLOROPHENOL
183.	PENTA	PENTACHLOROPHENOL
184.	PENTACHLOROPHENOL	PENTACHLOROPHENOL
185.	1-PENTANOL	n-AMYL ALCOHOL
186.	PENTYL ALCOHOL	n-AMYL ALCOHOL
187.	PERCHLOROETHYLENE	PERCHLOROETHYLENE
188.	PERCLENE	PERCHLOROETHYLENE
189.	PEROXIDE	HYDROGEN PEROXIDE
190.	PHENOL	PHENOL
191.	PHENOXY PESTICIDES	2,4-DICHLOROPHENOXYACETIC ACID
192.	PHENYLAMINE	ANILINE
193.	n-PHENYLANILINE	DIPHENYLAMINE
194.	PHENYLETHANE	ETHYLBENZENE
195.	PHENYLMETHANE	TOLUENE
196.	PHOSPHORIC ACID	PHOSPHORIC ACID
197.	PHOSPHORUS	PHOSPHORUS
198.	PHOSPHORUS WHITE	PHOSPHORUS
199.	POLYCHLORINATED BIPHENYL	POLYCHLORINATED BIPHENYL
200.	POLYFORMALDEHYDE	PARAFORMALDEHYDE
201.	POLYOXYMETHYLENE	PARAFORMALDEHYDE
202.	1-PROPANOL	n-PROPYL ALCOHOL
203.	PROPENAMIDE 50%	ACRYLAMIDE
204.	2-PROPENENITRILE	ACRYLONITRILE
205.	PROPYL ALCOHOL	n-PROPYL ALCOHOL

INDEX	SYNONYM	CHEMICAL NAME
206.	n-PROPYL ALCOHOL	n-PROPYL ALCOHOL
207.	PROPYLENE OXIDE	PROPYLENE OXIDE
208.	QUICKLIME	CALCIUM OXIDE
209.	SANTOPHEN 20	PENTACHLOROPHENOL
210.	SODIUM CYANIDE	SODIUM CYANIDE
211.	SULPHUR CHLORIDE	SULPHUR MONOCHLORIDE
212.	SULPHUR DIOXIDE	SULPHUR DIOXIDE
213.	SULPHURETTED HYDROGEN	HYDROGEN SULPHIDE
214.	SULPHURIC ACID	SULPHURIC ACID
215.	SULPHURIC ACID SPENT	SULPHURIC ACID
216.	SULPHURIC CHLOROHYDRIN	CHLOROSULPHURIC ACID
217.	SULPHUR MONOCHLORIDE	SULPHUR MONOCHLORIDE
218.	SULPHUR SUBCHLORIDE	SULPHUR MONOCHLORIDE
219.	SUPEROXOL	HYDROGEN PEROXIDE
220.	TAR CAMPHOR	NAPHTHALENE
221.	TDI	TOLUENE-2,4-DIISOCYANATE
222.	TEL	TETRAETHYL LEAD
223.	TETRA ALKYL LEAD	TETRAETHYL LEAD
224.	TETRACAP	PERCHLOROETHYLENE
225.	TETRACHLOROETHYLENE	PERCHLOROETHYLENE
226.	TETRACHLOROMETHANE	CARBON TETRACHLORIDE
227.	TETRAETHYL LEAD	TETRAETHYL LEAD
228.	TETRAHYDRO-p-OXAZINE	MORPHOLINE
229.	TETRAHYDRO-2H-1,4-OXAZINE	MORPHOLINE
230.	TETRAMETHYL LEAD	TETRAMETHYL LEAD
231.	TITANIC CHLORIDE	TITANIUM TETRACHLORIDE
232.	TITANIUM TETRACHLORIDE	TITANIUM TETRACHLORIDE
233.	TML	TETRAMETHYL LEAD
234.	TOLUENE	TOLUENE
235.	2,4-TOLUENE DIISOCYANATE	TOLUENE-2,4-DIISOCYANATE
236.	TOLUENE-2,4-DIISOCYANATE	TOLUENE-2,4-DIISOCYANATE
237.	TOLUOL	TOLUENE
238.	TOXILIC ANHYDRIDE	MALEIC ANHYDRIDE
239.	1,1,1-TRICHLOROETHANE	1,1,1-TRICHLOROETHANE
240.	TRICHLOROETHANE	1,1,1-TRICHLOROETHANE

INDEX	SYNONYM	CHEMICAL NAME
241.	TRICHLOROETHENE	TRICHLOROETHYLENE
242.	TRICHLOROETHYLENE	TRICHLOROETHYLENE
243.	TRICHLOROMETHANE	CHLOROFORM
244.	TRICLENE	TRICHLOROETHYLENE
245.	2,4,4-TRIMETHYL-1-PENTENE	DIISOBUTYLENE
246.	TRIOXYMETHYLENE	PARAFORMALDEHYDE
247.	UNSLAKED LIME	CALCIUM OXIDE
248.	VAM	VINYL ACETATE
249.	VANADIC ANHYDRIDE	VANADIUM PENTOXIDE
250.	VANADIUM PENTAOXIDE	VANADIUM PENTOXIDE
251.	VANADIUM PENTOXIDE	VANADIUM PENTOXIDE
252.	VCL	VINYL CHLORIDE
253.	VCM	VINYL CHLORIDE
254.	VINEGAR ACID	ACETIC ACID
255.	VINYL ACETATE	VINYL ACETATE
256.	VINYL A MONOMER	VINYL ACETATE
257.	VINYL CHLORIDE	VINYL CHLORIDE
258.	VINYL C MONOMER	VINYL CHLORIDE
259.	VINYL CYANIDE	ACRYLONITRILE
260.	VYAC	VINYL ACETATE
261.	WHITE CYANIDE	SODIUM CYANIDE
262.	WHITE PHOSPHORUS	PHOSPHORUS
263	XYLENES	XYLENES
264.	XYLOLS	XYLENES
265.	DIMETHYLBENZENES	XYLENES
266.	YELLOW PHOSPHORUS	PHOSPHORUS

II. FIRE HAZARD CODE

1. Flammable.
2. Not flammable.
3. Combustible.
4. Vapour may explode if ignited in an enclosed area.
5. Irritating vapours generated.
6. Poisonous and toxic vapours are produced when heated.
7. Flashback along vapour trail may occur.
8. Vapour is heavier than the air.
9. Toxic oxides of nitrogen may form in fire.
10. Highly flammable liquid.
11. Poisonous gases (Hydrogen Cyanide and Nitrogen Oxides).
12. Presence of oil or other combustible materials increases fire hazard.
13. Emits toxic fumes when heated.
14. Emits toxic fumes on decomposition.
15. Irritating gases generated in fire.
16. Toxic and irritating gases are produced in fire.
17. Containers may explode in fire.
18. Can react with oxidizing material.
19. May cause fire on contact with water and combustibles.
20. Decomposes to carbon monoxide and hydrogen cyanide in fire.
21. Toxic gases are generated.
22. Poisonous and irritating phosgene, chloride and hydrogen chloride gases are produced in fire.
23. May ignite on contact with air.
24. Flammable toxic vapours and poisonous gases are generated in fire.
25. Vapour forms explosive mixture with air.
26. Emits highly toxic fumes when heated to decomposition.
27. Toxic and irritating phosgene gas produced in fire.
28. If mixed with air in critical proportions and in presence of a source of fire, it ignites.
29. Reacts with metals vigorously such as aluminum and magnesium.
30. Toxic and irritating hydrogen chloride and phosgene gases are produced in fire.

31. Irritating vapours are produced when heated.
32. Toxic vapours are generated.
33. Toxic vapours are generated in fire.
34. Flammable gas may be produced on contact with metal.
35. Toxic and irritating chloride vapour produced when heated.
36. Toxic and irritating fluoride vapour produced when heated.
37. Flammable and explosive hydrogen gas produced on contact with metals.
38. Pressurized container explodes and releases toxic and irritating vapours.
39. Causes fire and explodes on contact with combustibles and metals.
40. Toxic oxides of sulphur produced in fire.
41. Dust cloud may be ignited by spark or flames, generating heat and toxic fumes.
42. Toxic and irritating fumes of nitrogen oxides produced when heated.
43. Black smoke, toxic fumes and gases including oxides of carbon and nitrogen are produced when burning in air.
44. Releases flammable and toxic formaldehyde vapours.
45. When heated, forms formaldehyde gas and oxides of carbon.
46. Poisonous gases produced in fire.
47. Poisonous and irritating gases of oxides of phosphorous are produced in fire - forms intense white smoke.
48. Releases highly hazardous cyanides when heated to decomposition or on contact with acid or acid fumes.
49. Container may rupture and release toxic and irritating sulphur dioxide.
50. Toxic and corrosive fumes of chloride and sulphur oxide are produced when heated.
51. Highly toxic fumes of lead produced in fire.
52. Reacts vigorously with oxidizing material.
53. Will increase intensity of fire when in contact with combustibles.
54. Toxic gases of hydrogen chloride, phosgene and carbon monoxide produced in fire.

III. REFERENCES

J. Chong

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